# **ChemSTEER User Guide**

# Chemical Screening Tool for Exposures and Environmental Releases



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# Introduction

# BACKGROUND AND PURPOSE OF CHEMSTEER

The Chemical Screening Tool for Exposures and Environmental Releases (ChemSTEER) is a computer-based software program developed by the U. S. Environmental Protection Agency (EPA) Office of Pollution Prevention and Toxics (OPPT) that can be used to conduct a screening-level workplace exposure and release assessment. ChemSTEER generates screening-level estimates for environmental releases of and worker exposures to a chemical manufactured and used in industrial and commercial operations (i.e. workplaces). The tool also contains data and estimation methods to assess chemical use in common industrial/commercial sectors (e.g., automotive refinishing) and chemical functional uses (e.g., tackifier in adhesive). ChemSTEER does not contain methods for estimating exposures to chemicals to the general public, to consumers, or to other species in the environment.

ChemSTEER was developed for technically knowledgeable users to support the EPA in assessing the potential exposures and risks to chemicals. A primary application is for assessing new chemicals that are submitted to EPA under Section 5 of the Toxic Substances Control Act (TSCA). Estimates from screening-level exposure models are not used as the sole justification for regulatory decision-making at EPA. When available, additional information, data, and more rigorous tools are used to improve the estimates of exposures and risks for such decisions. Another primary application is for assessing existing chemicals, such as those chemicals covered under the High Production Volume (HPV) Program, for which monitoring data are insufficient or unavailable. However, the use of ChemSTEER is not intended as a substitute for the collection and reporting of environmental and human health monitoring data.

ChemSTEER's methods and models are primarily intended to assess common sources of workplace releases and activities with worker exposure potential that are specific to a particular industry (e.g., overspray from auto body refinishing, textile dye bath dump, etc.) and other sources of workplace releases and activities with worker exposure potential that are "broadly applicable" across many workplaces (e.g., drumming semi-volatile liquid, scooping/weighing small volumes of powders, etc.). The "broadly applicable" sources/activities available in ChemSTEER are only a subset of all possible sources and activities and cover the sources/activities that are often overlooked or considered to be non-routine or insignificant. The methods and models in ChemSTEER have undergone internal EPA review and most have been used extensively in EPA assessments for over 10 years.

# **CURRENT/FUTURE VERSION INFORMATION**

The current version was developed primarily for preparing internal EPA reports on workplace releases and exposures. EPA has included several recent improvements over initial prototypes. These improvements are part of a continuing effort toward making ChemSTEER more "user friendly" for non-EPA users. Improvements and changes from the last publicly available versions (July 2003 Beta and May 2004 Beta include:

- Upgraded source code from Visual Basic 6 Platform to VB.NET platform.
- Updated layout of main screens, including numbering to facilitate easier navigation.

- Allow users direct access to specific EPA/OPPT models without starting an assessment (see <u>Direct Model Access (for Advanced Users)</u>
- Additional functionality to allow users to import operations from pre-defined Generic Scenarios or other assessments (see <u>Import Operations</u>)
- Addition of EPA/OPPT Solids Transfer Dust Loss Model
- Revised <u>EPA/OPPT Automobile OEM Coating Overspray Loss Model</u> and <u>EPA/OPPT</u> <u>Automobile Refinish Coating Overspray Loss Model</u> based on the June 2010 Emsision Scenario Document on Coating Application via Spray Painting in the Automotive Refinish Industry
- Updated Dermal Exposure Models for exposures to liquids according to the September 2013 updates to CEB's Method for Screening-Level Estimates of Dermal Exposure
- Revamped User Guide and Quick Start Guide
- Added/revised several Generic Scenario operations see "What's New section of the ChemSTEER application for complete list

EPA has the goal of developing future versions that will include additional improvements over the current version. These improvements will continue the effort toward making ChemSTEER more user friendly for non-EPA users. The future versions are envisioned to contain more methods (beyond defaults), improved terminology, fixes to any issues and problems, additional industry-specific operations and models, more output options (other text formats), and other improvements to enhance effectiveness and efficiency of the use of the software.

# LOGIC AND LAYOUT INFORMATION

## **Program Purpose**

ChemSTEER generates screening-level estimates for environmental releases of and worker exposures to a chemical manufactured and used in industrial and commercial operations (workplaces).

## Prerequisites

You must have a good understanding of the workplaces to be assessed (except for some specific industries programmed as "industry-specific operations" in ChemSTEER) and have some key chemicaland operation- specific data (e.g., vapor pressure, molecular weight, water solubility, throughput volumes, concentrations). You must also have a good working knowledge of ChemSTEER and its methods to generate credible results.

## Brief on the Logic of ChemSTEER

The current draft version was developed primarily to meet the objective of preparing internal EPA reports on workplace releases and exposures. The logic and layout of the program were developed to achieve this objective.

ChemSTEER functions by associating release sources and exposure activities expected for each type of workplace to particular EPA methods to estimate amounts (quantities) of release and exposure.

These methods may be scientific models, empirical methods, correlations, or presumptive methods (e.g., exposure will not exceed an OSHA PEL). Each method is based on an equation or set of equations containing parameters related to chemical- and operation-specific factors.

# The Layout of ChemSTEER

ChemSTEER is designed for you to enter input information in each tab and subtab, moving from the top-most tab to the bottom-most tab, and left-most subtab to the right-most subtab. It is recommended that you proceed with your assessments in this fashion, as some parameter values "flow down" through the assessment and are used as default values in subsequent pages. In other words, values that are entered in earlier tabs (those farther to the top) may be necessary inputs to later tabs (those farther to the top). Within each tab, values that are entered in earlier subtabs (those farther to the left) may be necessary inputs to later subtabs (those farther to the right). Main tabs and subtabs are numbered for ease of navigation.

The ChemSTEER program window contains eight main input pages (views) that can be accessed using the tabs at the left of each main page. The purpose of each of these main pages is described briefly below.

*General page (first tab)* - Record and view general information about the assessment on this page.

*Chemical page (second tab)* - Record and view information and data about the chemical being assessed on this page. The information and data include chemical identity-related information, assessment volumes, relevant physical/ chemical properties, use descriptions, and relevant regulatory information.

*Operations page (third tab)* - Record and view the types of operations ("homogeneous" workplaces - either user-defined or industry sector-specific) to assess, the immediate (direct) suppliercustomer relationship(s) each has to the other selected operations, the fraction of assessed volumes designated for each operation, and site identification information. For each operation selected, you must also verify or select the release sources and exposure activities. Some sources/activities are specific to a particular industry (e.g., overspray from auto body refinishing or textile dye bath dump), while other sources/activities are "broadly applicable" across many workplaces (e.g., drumming semi-volatile liquid or scooping/ weighing small volumes of powders). The broadly applicable source/activities available in ChemSTEER are only a subset of all possible sources and activities and cover those that are often overlooked or considered to be non-routine or insignificant. Each selected source/activity activates one or more equations that represent methods and models to quantify the release and/or exposure estimate(s).

*Operation Parameters page (fourth tab)* - For each operation selected, record and view key mass balance and container-related information used in the methods and models to estimate workplace exposure and environmental releases. This tab also contains other model parameters that are used by more than one release/exposure model (in the Shared Parameters/Factors subtab).

*Releases page (fifth tab) and Exposures page (sixth tab)* - For each source/activity selected under each operation included in the assessment, verify the use of the default estimation method(s) or select another method(s). For each selected method, verify and/ or enter values for parameters used by the

selected estimation method. After ChemSTEER has generated estimates of releases or exposures for an operation, you may combine amounts of releases from more than one source that are discharged to a particular media on the same day. You may also combine amounts of exposures from more than one activity that are potentially available to certain worker groups.

*Optional Information page (seventh tab)* - Record and view additional information relevant to the assessment, including information related to EPA assessments, the chemical's MSDS, pollution prevention information, general assumptions, and other information.

*Reports (eight tab)* - After ChemSTEER has generated release or exposure estimates, output page views become available from the Reports screen. In these views, ChemSTEER presents a final result overview based on the inputs, methods, and parameters selected. ChemSTEER also displays combined releases, as well as itemized exposures on these pages after you complete all relevant data inputs and click on the "Run Models" buttons on the Releases and Exposures tabs. Additional options available from the output page view windows include saving the output results to a text file and printing the results overview pages to a printer.

# LIST OF CURRENT KNOWN ISSUES

The following issues have been encountered while using the current version of ChemSTEER, but have not been able to be reproduced consistently:

- When switching quickly between tabs and various operations, the sources and activities for one operation may be come overlaid on to another operation. If this error is found before the assessment has been saved, go to the "Operations" tab and click between operations several times until the sources/activities are restored. If the assessment has been saved, the original sources/activities will be overwritten and lost.
- When opening an assessment and viewing the "Estimating Chemical Releases" or "Estimating Chemical Exposures" tabs, there is sometimes a "view error" where the model parameters do not appear for the selected operation and model.
- If a set operations is defined in a manner that creates a circular relationship, ChemSTEER may shut down when editing certain parameters, such as shared parameters on tab 4c.

# WHEN TO USE CHEMSTEER

ChemSTEER should be used when release and worker exposure data are not available but some estimates of these data are desired. Using ChemSTEER requires basic information about the chemical to be assessed; including amounts (in kilograms) of the chemical handled and used, key physical-chemical properties, and general information on how the chemical is manufactured, processed, and used. Using ChemSTEER also requires a basic understanding of both the processes used at a particular workplace (also called an "operation") and the available estimation methods within the tool.

ChemSTEER does contain some common industrial/commercial operations (also called "generic scenarios"), each of which is defined by a default set of processes. The operations contained in the tool are described in more detail in the <u>Operations Tab</u> section.

ChemSTEER is appropriate for use as a screening-level tool to assess potential chemical discharges to air (stack or fugitive releases), water, landfill, or incineration from operations. ChemSTEER can also be used to estimate potential worker inhalation and/or dermal exposures to chemicals in the operation. ChemSTEER may be run for a single type of operation or for multiple operations that may constitute part or all of the lifecycle of the chemical in workplaces.

# **INAPPROPRIATE USE AND LIMITATIONS OF CHEMSTEER**

Many models in ChemSTEER are characterized by EPA to be "screening-level." Screening-level results are intended to be conservative in that predicted results are likely to be higher, or at least higher than average, as compared to actual releases and exposures occurring in the real world setting. Some models in ChemSTEER, described as "what-if" models, are considered to be plausible, but whether their results are conservative are not known. If the exposure estimated by ChemSTEER is found to result in an unacceptably high health risk, then an appropriate next step in the assessment process is to verify and/or refine the parameter inputs and/or to perform the assessment with different and perhaps more complex models. Another response might be to consider monitoring to confirm results of the model.

ChemSTEER is also not appropriate for use when information about the chemical to be assessed, including amounts (in kilograms) handled and used, several physical-chemical property parameters, and some information on how the chemical is used are not known or well-understood. ChemSTEER is also not appropriate when the user does not have a good technical understanding of the processes used at a particular workplace (also called an "operation") and of the estimation methods used by the tool. ChemSTEER does contain some common industrial/commercial operations (also called "generic scenarios") each of which is defined by a default set of processes.

ChemSTEER does not estimate physical-chemical properties; environmental fate parameters; exposures to the general population, to consumers, or to the environment; or releases from or worker exposures to chemicals and products that are not covered under TSCA. If measured physical-chemical data do not exist, commercially available estimation software can be used to estimate these properties. Exposures to the general population, to consumers, or to the environment can be estimated using the Exposure, Fate Assessment Screening (E-FAST) tool, which is publicly available from EPA. E-FAST may be downloaded from the EPA Internet site at the following address: http://www.epa.gov/opptintr/exposure.

The releases estimated by ChemSTEER are expressed as the amount of the chemical per time discharged to various environmental media. The worker inhalation exposures estimated by ChemSTEER are expressed in average concentrations, potential daily dose rates, and lifetime-average daily dose rates, among others. The worker dermal exposure estimates for the chemical are also expressed as potential daily dose rates and lifetime-average daily dose rates, among others. ChemSTEER does not estimate absorption of the chemical by the human body.

This version of ChemSTEER contains most of the primary methods and models used by EPA. However, many of the industry/commercial sector-specific methods and models have not been included in this version. This version was developed specifically to meet EPA needs for assessing chemicals in data-sparse situations, although some considerations for external review and use of ChemSTEER were made. EPA is interested in specific suggestions for improvements on the methods and models and on the clarity of documentation for consideration in future updated versions. Feedback on improving ease of use and user-friendliness may also be considered given availability of resources.

# SOURCES OF METHODS AND MODELS IN CHEMSTEER

The methods and models used in ChemSTEER are from several EPA sources, including the "Chemical Engineering Branch Manual for the Preparation of Engineering Assessments" and other reports and memoranda detailing the methods used in CEB assessments. References to the industryspecific operations are taken from the "Chemical Engineering Branch Compilation of Generic Scenarios for Chemical Uses." These references document the various empirical, mathematical, and suppositional methods and models that have been developed and used by EPA over many years of workplace exposure and release assessment.

To review a complete list of references used in ChemSTEER, go to the <u>References</u> section of this User Guide.

# **ABOUT THIS VERSION AND PROVIDING FEEDBACK**

This version has been developed for internal EPA use and testing. EPA has released this version to allow interested parties to view the tool's current status, to better understand EPA's workplace exposure assessment methods, and to provide suggestions on improving methods and models and other features of the tool.

Over the past several years, ChemSTEER has been undergoing continuous updating as minor features are changed and new features are added, particularly industry-specific operations (scenarios for particular formulation or use applications). Also note that this version has received limited testing before it became publicly available.

Any version that was found to have significant problems during testing (e.g., creates instability on the host PC, "crashes" easily, or gives incorrect outputs) has not been released. This version has been released because it has already been committed to routine use for generating internal EPA assessments and reports. Among about 20 versions over the past several years, only a few prior versions have met the standards for on-going internal use and public release.

EPA is interested in gaining feedback from non-EPA users on the usefulness of ChemSTEER. EPA will consider specific suggestions for improving the methods and models or for improving the user-friendliness in future updates of the tool.

Please send your feedback and suggestions to the contact listed at the bottom of the ChemSTEER home page at: <u>http://www.epa.gov/opptintr/exposure/pubs/chemsteer.htm</u>.

The most recent version of ChemSTEER and additional exposure-related information and resources are available from the following EPA Internet sites: <u>http://www.epa.gov/opptintr/exposure/pubs/chemsteerdl.htm</u> and <u>http://www.epa.gov/opptintr/exposure/pubs/guidance.htm</u>.

# **Getting Started**

# **CHEMSTEER HARDWARE REQUIREMENTS/SOFTWARE ISSUES**

## Hardware & Software Requirements

- Windows XP or above
- Processor minimum recommended for your version of Windows
- Memory minimum recommended for your version of Windows
- Hard disk space minimum recommended for your version of Windows

# **Screen Resolution**

ChemSTEER is designed for a screen resolution of at least 1024 x 768 pixels with 96 dots per inch (DPI) or less. You can also run ChemSTEER with a lower screen resolution or higher DPI; however, some information and buttons will not be visible. You may not be able to navigate off of a window because buttons may not be visible on your screen. It is not recommended to run ChemSTEER with a screen resolution lower than 1024 x 768 pixels and higher than 96 DPI. To change your resolution, right-click on your main Windows window, select Properties, select the Settings tab to select the desired screen resolution, and click OK. To change your DPI, right-click on your main Windows window, select Properties, select the Advanced button, and select your DPI setting.

# WHAT YOU NEED TO USE CHEMSTEER

- Understanding of the purpose, limitations, and methods in ChemSTEER;
- Information and data (properties, amounts, and uses) about the chemical to be assessed; and
- Site-specific information about the workplaces handling the chemical (except for some industrial or commercial workplaces for which default information and parameters are available in ChemSTEER).

To effectively and properly use ChemSTEER, you must first understand the purpose and limitations of ChemSTEER. These are discussed in the <u>Introduction</u> section of this User Guide.

You must understand the terminology in ChemSTEER. The <u>Definitions and Terms</u> section of this User Guide can be used to clarify and understand ChemSTEER terminology.

You must also understand the <u>ChemSTEER Estimation Methods and Models</u> used to generate workplace exposure and release estimates. This understanding is needed to effectively determine whether the best and most appropriate model is used for each release and exposure to be estimated.

You must have access to certain information about the chemical to be assessed. Some methods and models used in ChemSTEER require physical-chemical property parameters. Vapor pressure, mole fractions, densities, and water solubility are the parameters most commonly used in the ChemSTEER models and methods. Also, you must provide the amount (in kilograms) of the chemical that is manufactured or imported, processed or used within the scope of the assessment. When multiple

workplace operations are to be assessed, you must provide the relationship of supplier-customer operations and should provide a best estimate of the fraction of the amount that is devoted to each operation assessed.

# **GENERAL TIPS AND NOTES FOR USING CHEMSTEER**

You should read the User Guide thoroughly. Understanding the various functions in the software is crucial to the effective use of ChemSTEER and its models. It is especially recommended that you review the following sections of the User Guide:

- <u>Chemical Properties Tab</u>, particularly noting the required inputs;
- Operations Tab  $\rightarrow$  Relationships Subtab;
- <u>Operations Tab → Sources/Activities Subtab;</u>
- Each of the subtabs within the **Operations Parameters Tab**; and
- <u>ChemSTEER Estimation Methods and Models</u>.

Pay particular attention to the bases and sources of the default values used in the above calculations and logic, as well as where they may be used elsewhere in the assessment.

The buttons for each main screen are listed on the left side of the application and should typically be completed sequentially. Within each screen, the user should generally complete pages (subtabs) sequentially from left to right because some parameters' values "flow down" through the assessment and are used as default values in subsequent pages. In other words, values that are entered in earlier pages (those farther to left) may be necessary inputs to later pages (those farther to right). Review the <u>Hierarchy of ChemSTEER Operations, Activities, and Models</u> section below for more information.

New users may wish to review the *ChemSTEER Quick Start Guide* (included with this version of ChemSTEER) and any other training guides available on EPA's website: <a href="http://www.epa.gov/opptintr/exposure/pubs/chemsteer.htm">http://www.epa.gov/opptintr/exposure/pubs/chemsteer.htm</a>.

You should understand the *File* menu options for using *Save* and *Save As* to maximize preservation of data. For example, using *Save* overwrites data for the assessment in the ChemSTEER database file, while *Save As* saves the information to a new file. In addition, saving multiple assessments to a single ChemSTEER database file will use less disk space than saving single assessments each to a separate database (i.e., creating multiple ChemSTEER database files) (see <u>Saving Your Assessment</u>).

You may enter values in either decimal format (e.g., 5423.78 or 0.00267) or in scientific notation (e.g., 5.42378E03 or 2.67E-03 or 2.67E-3). <u>ChemSTEER will not accept</u> exponential scientific notation format (e.g., 5.42378 x 10^3 or 2.67 x 10^-3).

ChemSTEER also does not currently accept number qualifiers, such as "<" or "=>". It is recommended that you capture information such as this in the *Basis* sections found wherever values are entered. Review the <u>Storing and Displaying Values within ChemSTEER</u> section below for more information.

ChemSTEER contains several Basis text boxes located throughout the assessment in order for you to provide additional information on the particular input values and general assumptions used in the assessment. You are strongly encouraged to use these Basis boxes.

NOTE: Any carriage return entered within these boxes will appear as a "|" within the text when an existing assessment is opened and viewed within ChemSTEER. These carriage returns "|" will also appear in the reports generated by ChemSTEER.

If you wish to assess volatile releases or inhalation exposures to vapors, be sure that the substance you are assessing has an adjusted vapor pressure within the specified range for the vapor generation models. The default range is between 0.001 and 35 torr. If you wish to modify the range, go to the *Preferences* menu and select <u>Vapor Model Activation</u>.

Note that the *Mass Balance Inhalation Model* uses some parameters from an associated vapor generation release model as default values in calculating inhalation exposure. If you plan to use the *Mass Balance Inhalation Model*, be sure to use the appropriate release model for vapor generation, and be sure that the release model is in the appropriate place (last) on the list of release models for the source/activity (see <u>EPA/OPPT Mass Balance Inhalation Model</u>).

# HIERARCHY OF CHEMSTEER OPERATIONS, ACTIVITIES, AND MODELS

ChemSTEER assessments have a hierarchical organization of operations, activities, and models. Assessments contain one or more operations. Operations contain one or more activities. Activities may contain one or more models.

When models are run on either the Releases or Exposures tab, all of the models within the selected operation are run. Similarly, when Operations are analyzed in the IRER report, all of the activities and models within each operation are processed and analyzed as a unit.



This hierarchy of operations, activities, and models has several significant implications on how ChemSTEER operates and how interrelated elements of an assessment are affected when you make a change:

- When Operations are deleted, all of the activities and models within the operation are deleted.
- When an Activity is deleted, all of the models within the activity are deleted.

ChemSTEER also has an information hierarchy, as shown below. The information hierarchy is significant because information only 'flows down' to non-user-specified parameters at lower tiers. For example, Molecular Weight in the Chemical Information tier flows down to Molecular Weight in the Operation Information tier (Shared Parameters) and then to Molecular Weight in the Model-Level Information tier. Molecular Weight entered in the Operation Information tier would only flow down to the Model-Level Information tier.



The sections below describe how UPDATING particular parameters in an assessment affect other parameters and functions within ChemSTEER.

# Updating Total Assessed PV on the Chemical Tab or Assessed PV on the Relationships Tab

If you update the Total PV on the Chemical tab, ChemSTEER will update the Production Volume for each Operation (PVop) based on the existing Fraction of Production Volume (PVf) for each operation for all operations. If you update the existing Fraction of Production Volume on the Relationships tab, the PV for the operation will be updated.

For each operation that changed PV, you must click the *Update Parameters* button (on the Mass Balance Parameters subtab of the Operation Parameters tab) and click *OK* or *Calculate remaining two parameters* in the Specify Mass Balance Input Parameters subtab. When you update the PV, ChemSTEER will notify you that you must complete the Mass Balance Input Parameters. You will be prevented from saving or running models until you do so.

Clicking *OK* or *Calculate remaining two parameters* will re-calculate the Mass Balance Input Parameter values based on the new PVop using the following methods:

- 1. The remaining two parameters will be recalculated using current user-specified check boxes for the five primary mass balance parameters (shown in the *Specify Mass Balance Input Parameters* subtab).
- 2. Any of the other mass balance parameters (displayed at the bottom of the *Specify Mass Balance Input Parameters* subtab) that are not user-specified will be recalculated using the updated PVop.
- 3. If you have a batch operation and the number of batches per year (Nby) has changed because of the new PVop, the non-user-specified daily batch parameters on the *Specify Other Batch Parameters* subtab will be re-calculated.

See the <u>Updating Mass Balance Values</u> section below for more information on updating calculated values.

# Updating Chemical Vapor Pressure (VPchem) and Molecular Weight (MW) on the Chemical Tab

The vapor pressure (VPchem) and molecular weight (MW) from the Chemical tab are used by certain models, as well as in the calculations performed on the Shared Parameters subtab of the Operation Parameters tab (e.g., VPchem is used in the calculation of AVPlow and AVPhigh; MW is used in the calculation of the mole fractions (i.e., Xrm, Xprod, or Xother) using Raoult's law).

When you update VPchem and/or MW in the Update Chemical Information window and click the OK button, all non-user-specified values of VPchem and MW are automatically overridden in any model that utilizes these parameters.

In addition, the values of AVPlow and AVPhigh are updated for the new VPchem and mole fractions calculated by Raoult's law are re-calculated using the new MW.

The release and exposure models will also need to be re-run to reflect the updated values in VPchem, MW, and the mole fractions.

NOTE: The original default models for the sources/activities will not be changed, even if a model-defaulting conditional parameter has been changed as a result of the update. For example, if the original VPchem and resulting AVPprod were within the preferred AVPrange, then the *Loading Liquid Product into Drums* source/activity included *the EPA/OAQPS AP-42 Loading Model* as a default for calculating releases to air. If you then modify the VPchem such that the resulting AVPprod is now below the preferred AVPrange, the *EPA/OAQPS AP-42 Loading Model* remains associated with the loading source/activity (in a new assessment, if AVPprod were less than the preferred AVPrange, the *EPA/OAQPS AP-42 Loading Model* would not have been defaulted). You must remove the air release model manually if you no longer wish to assess volatile releases to air from the source/activity.

Refer to the following User Guide Topics for more information:

- Vapor Model Activation
- <u>Operation Parameters Tab → Shared Parameters/Factors Subtab</u>
- Default Model Processing

## Updating the Chemical Solubility in Water (WSchem) on the Chemical Tab

The chemical water solubility (WSchem) from the Chemical tab is not used in the Mass Balance, Container Parameters, or Shared Parameters subtab calculations (all within the Operation Parameters tab); however, it is used by some models. When you update WSchem and click the *OK* button in the Update Chemical Information window, all non-user-specified values of WSchem are automatically overridden in any model that utilizes WSchem in its calculations.

The release and exposure models will need to be re-run to reflect the updated value in the model outputs.

# Updating Chemical Density (Dchem) on the Chemical Tab

The chemical density (Dchem) is used in the Container Parameters subtab calculations (of the Operation Parameters tab). When you update Dchem and click the *OK* button in the Update Chemical Information window, Dchem automatically updates default densities in the Container Parameters input subtabs. In the Verify/Select Container Parameters by Source/Activity subtab, you should verify all user-specified container parameters and click the *Calculate the remaining two values* button or the *Restore Defaults* button to recalculate container parameters based on the new Dchem. See updating "Container Parameter Values" below.

# **Updating Mass Balance Values**

Clicking *Calculate remaining two parameters* on the Specify Mass Balance Input Parameters tab will re-calculate the "other" three mass balance parameters (displayed at the bottom of the Specify Mass Balance Input Parameters subtab) and the daily batch parameters on the Specify Other Batch Parameters subtab (if a Batch basis is selected for the mass balance calculations) according to the following rules:

- If none of the "other" mass balance parameter values and/or the daily batch parameter values are user-specified, those will be updated according to the default logic.
- If two of the "other" mass balance parameter values are user-specified, the third value will remain unchanged. You should re-verify those values.
- If only one of the "other" mass balance parameter values is user-specified, ChemSTEER will re-default the second value based on the primary five mass balance parameter values (shown at the top of the subtab), and will recalculate the third value based on the user-specified and re-defaulted value. It is recommended that you verify the user-specified "other" mass balance parameter value.

Clicking *OK* will return you to the Operations tab. NOTE: You may receive error messages to resolve mass balance discrepancies (e.g., the calculated operating days per year exceeds 365).

When you make updates to Mass Balance Parameter values and click the *OK* button (on the Update Operation Mass Balance Parameters window), the affected non-user-specified Container Parameter values are automatically recalculated. Note that in order for all Container Parameter values to be calculated, you must specify at least the appropriate Weight Fraction and the Number of Sites on the Mass Balance Parameters subtab. When user-specified container parameters are used, you should verify that the user-specified container parameters are still applicable and click the *Calculate the remaining two values* button to eliminate any possible discrepancy. For example, operating days (ODa) may have been calculated based on three other user-specified container parameters to be 100 dpy; however, because ODa is not user-specified, changing OD to 250 dpy on the Mass Balance parameters subtab would cause ODa on the Container Parameters subtab to update to 250 dpy, causing a discrepancy between the three user-specified container parameters.

Any non-user-specified model value associated with the modified Mass Balance parameter is automatically overridden in any model that utilizes the modified parameter in its calculations. The release and exposure models will need to be re-run to reflect these updated values in the model outputs.

Note: if you change Yprod in an operation and Yprod is used as the default value for Yrm in a subsequent operation, the Yrm will <u>not</u> be updated to the modified Yprod value from the previous operation – Be sure to click the *Restore Defaults* button in the subsequent operation(s) Mass Balance Parameter screen to allow the Yrm to be automatically updated with a modified Yprod from the previous operation. The release and exposure models in the subsequent operation will also need to be re-run to reflect the updated value in the model outputs.

## **Updating Container Parameter Values**

On the Container Parameters subtab, when user-specified container parameters are used in the Verify/Select Container Parameters by Source/Activity subtab and changes are made that affect the other parameters used in the calculations, you should verify that the user-specified container parameters are still applicable and click the *Calculate the remaining two values* button to eliminate any possible discrepancy between the parameters in the two Container Parameters subtabs.

When you make updates to container-related source/activity parameters in the Container Parameters subtab and click the *OK* button (on the Update Container Parameters window), all non-userspecified, container-related model parameter values are automatically overridden in any model that utilizes them in its calculations.

The release and exposure models will need to be re-run to reflect these updated values in the model outputs.

## **Updating Shared Parameter Values**

When you make updates to a value on the Shared Parameters subtab and click the *OK* button (on the Update Shared Parameters window), all non-user-specified, shared parameter model values are automatically overridden in any model that utilizes them in its calculations.

The release and exposure models will need to be re-run to reflect these updated values in the model outputs.

## **Updating Vapor Generation Rate Model Equation Parameters**

When the release of a volatile chemical is assessed in ChemSTEER, the release model calculates a vapor generation rate (G). This parameter is then used to calculate the daily release of the chemical to air. To read more about these types of release models, go to the <u>Models for Calculating Releases to Air</u> section of this User Guide.

The G parameter, as well as other model input parameters such as hours per day, that are calculated or set in the selected release model are then passed to and used by the <u>EPA/OPPT Mass</u> <u>Balance Inhalation Model</u> to calculate the corresponding worker exposure to the chemical vapor on the Exposures tab. If you change any of the input parameters for the air release model, you should re-run the release models in order to recalculate the G parameter. This will ensure that the most current input parameter values are passed to and utilized by the inhalation exposure model.

Review the <u>Calculating Two Sets of Results from a Single Model</u> section to read more about how the two sets input parameters (i.e., used to calculate Output 1 and/or Output 2 results) for each of the air release and inhalation exposure models work together.

## **Default Model Processing**

The sources/activities in ChemSTEER typically have one or more default release and/or exposure models associated with them. These default models may be conditional based on the input data values in the assessment. Default Model Processing (DMP) is the function in ChemSTEER that adds default models to the source/activity based on the conditions in the assessment.

For more information on which models are defaults for each source/activity, see <u>Release</u> <u>Sources and Exposure Activities</u>.

Default release models are selected for each source as soon as you select the operation on the Releases tab. Similarly, the default exposure models are selected for each activity when you select the operation on the Exposures tab. The default release and exposure models are added to each source/activity within an operation only once in an assessment. Once the operation is selected, any of the sources/activities within that operation that have not already been *processed for Default Models* will be processed to determine which default models are appropriate for each source/activity.

Once a source/activity has been 'processed' and the default models are set, that source/activity will not be 'processed' again. In other words, the original default models will not be changed, even if a conditional parameter has been revised. For example, if a vapor-generation model was selected by default as a result of the AVPlow/AVPhigh values, that model will not be de-selected if the parameter values are subsequently changed such that the VP for the chemical is less than AVPlow or greater than AVPhigh.

However, if new sources/activities are added to an operation, they will be 'processed' for default models based on the current criteria such as the AVPlow to AVPhigh range. This is true even if the operation contains sources/activities that were previously 'processed'.

The 'status' of Default Model Processing for each source/activity is shown on the Sources/Activities subtab located on the Operations tab. The *Release DMP* displays the status of the source/activity's release models and the *Exposure DMP* displays the status of the source/activity's exposure models. The four values for DMP are:

Pending	DMP has not yet been done on the source/activity
Cond Models Added	DMP has been done on the source/activity and conditional models were added
Cond Models Not Added	DMP has been done on the source/activity and conditional models were not added
No Cond Models	DMP has been done on the source/activity but it had no conditional models

You can always change default release or exposure models that ChemSTEER has chosen for a given source/activity. If you would like to either remove a model or replace a chosen model with a different model, click the *Add or Remove a Model* button on the Releases or Exposures tabs, as appropriate.

If you would like ChemSTEER to re-default models based on new conditions for a source/activity that has already been processed, in the Update Sources/Activities window on the Operations tab / Sources/Activities subtab you can:

- 1) Change the *Release* and/or *Exposure* status from Yes to No, click *OK*, and then return the status to Yes, or
- 2) Remove the activity from the list and then add the activity back to the list.

**NOTE:** either one of these methods will cause any user-specified values and outputs to be lost. You will need to re-enter any values that you had entered previously.

# STORING AND DISPLAYING VALUES WITHIN CHEMSTEER

# <u>Dates</u>

ChemSTEER uses the MM/DD/YYYY format for dates.

# **Rounding of Numbers**

- 1. If the digit to the right of the "rounding digit" is less than 5, the rounding digit is not changed but all digits to the right of it are dropped.
- 2. If the digit to the right of the "rounding digit" is greater than or equal to five, one is added to the rounding digit and all digits to the right of it are dropped.
- 3. When ChemSTEER rounds using the Scientific Notation function (described below), the display of your calculated or entered value may change; however, the exact value will still be retained in ChemSTEER and used in subsequent calculations

Exception: if a field is designated as a whole number (non-negative integer) and a decimal value is calculated, ChemSTEER will round any value below 1 to 1. For example, on the Mass Balance tab, if the Number of Sites (NS) is calculated based on other values to be 0.2, ChemSTEER would change NS to 1, but display a warning for an apparent mass balance discrepancy.

# **Display of Numbers using Scientific Notation/Significant Digits**

## **User-Entered Values**

Most user-entered values are saved as "Single" data types to save disk space and because users are not expected to enter values with an excessive level of accuracy. For these user-entered cases, ChemSTEER will convert the number to a Single data type. The General Number form typically stores and displays values as entered; however, Microsoft Access generally limits stored values to 8 characters (including the decimal point, but excluding the leading zero before a decimal point and the scientific notation E-00).

For example, if you enter 300.001 for MW on the Chemical tab, ChemSTEER will save and use that value. However, if you enter 300.345678, ChemSTEER will convert that value to 300.3457. Likewise, an entered VP of 0.000012345678 will be converted to 1.234568E-05.

## **Calculated Values**

ChemSTEER uses Single data types for calculated values. While ChemSTEER retains and uses the calculated values, the following rules (Scientific Notation function) are invoked for display purposes:

- 1) Numbers that are required to be non-negative integers (e.g., NS) are displayed as whole numbers.
- 2) All other numbers typically are displayed using the following rules:
  - If the number if > 100, it is displayed with the format of ###,##n.##

(e.g., 190.1 displays as 190.1, 190.001 displays as 190, 5 million displays as 5,000,000)

• If the number is > 0.1 and <= 100 then it is displayed as ###,##n.#####

(e.g., 90.01 displays as 90.01, .55555 displays as 0.5556)

• If the number if > 0.01 and <= 0.1 then it is displayed as 0.###

(e.g., 0.055555 displays as 0.056)

 If the number is > 0.1E-15 and <= 0.01 it is displayed as 0.0000E-nn (e.g., .00555555 displays as 5.5556E-03)

Note: "#" will cause any leading or trailing zeros to be removed; "n" displays the numeric digit even if it is zero.

The following table shows when the Scientific Notation function is used.

Window/Tab	Usage of Scientific Notation Function
Chemical tab	No
Chemical Update Window	No
Operations Parameters (Relationship tab)	Yes (however, Pvop for the current operations will not display if < 0.001)
Operations Parameters (Relationships update window)	No
Mass Balance tab	Yes (except for parameters that are required to be integers, like OD, NS, LS, etc.; and Nbld, which is set to one fixed digit after the decimal point)
Mass Balance update window	No
Container Parameters tab	Yes
Container Parameters update window	Yes (except when Restore Defaults is used)
Shared Parameters tab (X/A VP)	Yes
Shared Parameters update window (X/A VP)	No
Release Model Input Parameters tab	No
Release Model Input Parameters update window	Νο
Exposure Model Input Parameters tabs	No
Exposure Model Input Parameters update window	No
Exposure Model Output tab	Yes

# **COMPLETING COMPREHENSIVE ASSESSMENTS**

To use ChemSTEER effectively and efficiently, you should enter all information and parameters that cause ChemSTEER to populate default parameters' values for the models that you plan to use.

You should generally enter information and data within each page from left to the right. This is because some parameters values in tabs to the right originate or are calculated from parameter values in earlier (left) tabs. The following process is generally recommended for most new assessments:

Initiate ChemSTEER, or if you are viewing or using an assessment, save that assessment if desired, then click *File/New Assessment*, which will clear all information and data entered in the previous assessment from all views. Begin by entering any information that you may want to record on the *General* tab. You should be sure to enter an Identifier.

Click on the *Chemical* tab and enter assessment volume(s) and chemical properties parameters' values.

Click on the *Operations* tab and first select all operations to assess. This selection is completed on the window accessed using the *Update Operations* button. Then for EACH operation selected and in the order selected, complete the data fields for each of the subtabs as they are ordered from left to right (Relationships, Description, Physical States, Source/Activities, and Site Information). Note: you may include up to 20 sources/activities within each operation that is assessed in ChemSTEER.

Click on the Operation Parameters tab.

For EACH operation, enter the *Mass Balance* subtab parameters accessed using the *Update Parameters* button. Then click on the *Container Parameters* subtab.

For EACH operation, view the *Container Parameter* subtab parameters in each of the subtabs as they are ordered from left to right (For Raw Materials, For Other Materials, For Product, and Container Parameters by Activity). If you wish to change any of the parameters' values, double-click on the appropriate Source/Activity name and make the change. Finally, click on the *Shared Parameters/Factors* subtab.

For EACH operation, review the model parameters that are shared between more than one model. Currently, this subtab allows you to adjust the vapor pressure of the raw material, product, or other material. You can also select parameters for the Automotive Spray Coating models in this subtab.

Click on the *Releases* tab. For each Operation, check each Release Activity first by determining whether the Release Models are those that you want to use. Change models if desired, and then for each Model check the parameters used in the models and, if needed, click the *View/Update Model Information* button to change any parameter values that need to be updated. Click *Run Model(s)* and click on the *Estimated Releases* subtab to view model outputs. You may change the medium/media of release by clicking on the *Modify Media of Release* button.

Click on the *Exposures* tab. For each Operation, check each Exposure Activity first by determining whether the Exposure Models are those that you want to use. Change models if desired, and then for each Model check the parameters used in the models and, if needed, click the *View/Update Model Information* button to change any parameter values that need to be updated. *Click Run Model(s)* and click on the *Estimated Exposures* subtab to view model outputs.

Click on the *Optional Information* tab and enter any relevant information for any topic in the combo box.

Save your assessment. If you cannot finish the assessment in one sitting, you may Save the assessment at any point in its development, then later Open the assessment and continue where you had stopped.

Note: Be sure to use the Basis buttons to document key assumptions and data and to explain use of non-default values, particularly in the various update windows accessed from the *Operation Parameters, Releases, and Exposures* tabs.

# **DIRECT MODEL ACCESS (FOR ADVANCED USERS)**

This version of ChemSTEER has been developed to allow you to access specific environmental release or occupational exposure models directly from the Splash Screen or Menu bar. To access this function, click on the "Run Exposure/Release Models (Advanced Users)" on the splash screen or through

*File/Run Models (Advanced Users)* on the menu bar. It is recommended that you familiarize yourself with each model – see the following sections for a summary of each model:

- Quick Summary of ChemSTEER Release Models
- Quick Summary of ChemSTEER Inhalation Exposure Models
- Quick Summary of ChemSTEER Dermal Exposure Models

When the option is selected a popup screen allows you to select a single model from one of three categories: "Release Models", "Dermal Exposure Models", or "Inhalation Exposure Models". Once you have selected a model, click the Ok button. This takes you directly into ChemSTEER, directly to the appropriate "View/Update Model" screen. ChemSTEER will automatically set the model's parameter types to non-default. The user will be able to immediately enter parameter values and run the model as normally done during an assessment.

Once the selected model's parameters have been entered and the model has been run, the estimated releases or exposure will be available for viewing on the regular ChemSTEER screens. The user then has the option of preparing an assessment. If you wish to run a different model, you can select File/Run Models (Advanced Users)" from the file menu.

Note: For release models, the error message indicating that the release exceeds the PV will not be suppressed since users of this function are expected to be advanced and to avoid potential issues if the assessment is saved.

# Guide to the ChemSTEER Menus

# **FILE MENU**

## Starting a New Assessment

You may choose *File/New Assessment* to clear all ChemSTEER fields of a working assessment. Choosing *New Assessment* removes all data elements (selected operations and sources/activities; all parameters and associated information; and model estimates) from the ChemSTEER interfaces (i.e., screen views shown on your monitor) and from the ChemSTEER working assessment databases. This removed data and information cannot be retrieved unless it was saved to a file prior to choosing *New Assessment*.

# **Opening an Existing Assessment**

You may select *File/Open Assessment* to retrieve a previously saved Assessment (record) from an existing ChemSTEER database file.

If the existing database file contains only one Assessment record, the information in that record will appear in the ChemSTEER interface (screen views shown on your monitor).

If the existing database file contains more than one Assessment record, a table of Assessment records will appear that includes six fields in the record: Type, Fiscal Year, Identifier, Consolidated Case, Status, and Date. You may click on any of these fields or on the gray rectangle to the left of the 'Type' field in the row of the Assessment record that you wish to open. This will cause an arrow to appear in the gray rectangle in the row of Assessment record that you wish to open. Once this arrow is in the row of Assessment record that you wish to open button will cause the information in that record to appear in the ChemSTEER interfaces.

You may also use the Search button to filter available assessments by one or more of the following parameters: Assessment ID, Assessment Type, Assessment Status, or Date Range. If you wish change your selection criteria, you can delete entered text from the Assessment ID and Date Range text boxes and hit the reset button(s) to clear the Assessment Type and/or Assessment Status drop-down box(es).

## **Opening Assessments Created in an Earlier Version of ChemSTEER**

ChemSTEER allows you to open and modify assessments that were originally created and saved with an earlier version of the software. Any assessment that was created with the December 2003 version of ChemSTEER or later may be opened, reviewed, and/or modified using the current version. Note: The December 2003 version of ChemSTEER was created for internal testing/use and was not released to the public.

If you make changes to the previous assessment and wish to save these changes, you <u>must</u> select the *File* menu and click *Save Assessment As* to save it to the current version of the ChemSTEER database. You must also update the assessment to the current version of the database prior to running reports. See the <u>Saving Your Assessment</u> topic of the User Guide for more information.

## Attempting to Open an Assessment Using an Older Version of ChemSTEER

ChemSTEER will not allow you to open an assessment that was last saved in a more recent version of the software. For example, an assessment saved in an April 2, 2004 version of ChemSTEER may not be opened using a December 2003 version of the software. If you attempt to open a more recent assessment using an older version of the software, you will receive the following error message:

"Version Error: You have opened an assessment that was created in the [date] version of ChemSTEER. This is not permitted. Please use the later version of ChemSTEER to open this assessment."

Note: The December 2003 version of ChemSTEER was created for internal testing/use and was not released to the public.

# Saving Your Assessment

You should save your assessments frequently throughout their development. ChemSTEER has no automated backup feature, and saving frequently is one way to protect your data due to unanticipated program shutdown or power loss.

Assessments may be saved as individual records in a database file containing multiple records or as their own individual database files.

If you open an assessment (record) from an existing database file, you may view and/or edit the assessment on the ChemSTEER interfaces (screen views).

You may choose *File/Save Assessment* to overwrite the assessment that is in the existing database file with the working assessment that is displayed on the ChemSTEER interfaces; however, if the *identifying fields* in the current assessment are identical to the *identifying fields* of an assessment already in the database file, ChemSTEER will display the following message box:

"A duplicate assessment exists in the database. Do you want to replace the existing assessment with the current assessment? If not, you must change at least one Identifying Field."

Alternately, if you changed any of the identifying fields in the assessment since the last time you saved, ChemSTEER will display the following warning:

"You have changed an Identifying Field since your last save and continuing with the save will overwrite your existing assessment. If you wish to create a new assessment, you should Cancel and use Save Assessment As."

For a discussion of identifying fields, please see the <u>General Information Tab</u> topic.

NOTE: To save the assessment, click the Save button in the Save Assessment As dialog screen.

#### Saving Assessments before Mass Balance Parameters Have been Updated

If you have updated the PV or imported an operation into ChemSTEER, you are required to update the Mass Balance Parameters before saving. If you have not updated your mass balance parameters, you will receive a warning message when you attempt to save the assessment.

#### Saving Assessments Before All Models Are Run

If you have sources/activities included in your assessment and you have either never run the associated release or exposure models or have made changes to the settings or parameter values used by any of the selected models, you will receive a warning message when you attempt to save the assessment.

The warning message will display the models that are not current (i.e., have not been run). You may choose to:

- 1. *Run All Models* this option will cause ChemSTEER to proceed in running all of the models with their current settings and parameter values and save the assessment.
- 2. *Continue without Running All Models* this option will cause ChemSTEER to save the assessment without running the models.
- 3. *Cancel Action* will remove the "request" to save the assessment and will return you to your assessment.

#### Saving a Revised Assessment with a New Name

Alternately, you may choose *File/Save Assessment As* to create a new assessment record (i.e., the working assessment that is displayed on the ChemSTEER interfaces) either in an existing database file or a new database file. *Save Assessment As* prevents ChemSTEER from overwriting an existing assessment record that was retrieved from the existing database file and edited, however, if the *identifying fields* in the current assessment are identical to the *identifying fields* of an assessment in the destination database, ChemSTEER will display the following message box:

"A duplicate assessment exists in the database. Do you want to replace the existing assessment with the current assessment? If not, you must change at least one Identifying Field."

For a discussion of identifying fields, please see the <u>General Information Tab</u> topic.

When using *File/Save Assessment As*, ChemSTEER defaults the database save name according to the following convention:

[Assessment Type][Fiscal Year]-[Assessment Identifier]"C"{if the Consolidated Case = Yes} [Status]

NOTE: To save the assessment, click the Save button in the Save Assessment As dialog screen.

#### Saving Changes to an Assessment Created by an Earlier Version of ChemSTEER

ChemSTEER allows you to open and modify assessments that were originally created and saved with an earlier version of the software. Any assessment that was created with the December 2003 version of ChemSTEER or later may be opened, reviewed, and/or modified using the current version. Note: The December 2003 version of ChemSTEER was created for internal testing/use and was not released to the public.

If you make changes to the previous assessment and wish to save these changes, you <u>must</u> select the *File* menu and click *Save Assessment As* to save it to the current version of the ChemSTEER database. You must also update the assessment to the current version of the database prior to running reports.

If you click either *File/Save Assessment* or attempt to run a report before first saving the previous assessment to a current database, ChemSTEER will display the following warning:

"Version Warning: You have opened an assessment that was last saved in a previous version of ChemSTEER. You will need to do a *Save Assessment As* before running reports."

## Attempting to Save to a Full Disk

Each time you save your assessment, ChemSTEER checks your target location to determine if you have enough disk space for the assessment. If you try to save to a location with less than 2 megabytes (MB) of available space, ChemSTEER will display the following message:

"You have selected a save location with inadequate space for this assessment. Please select an alternative location (with more than 2 MB of available space) to save the assessment."

If you see this message, you must select another location to save the assessment.

# Replacing the Generic Scenario Database

This version of ChemSTEER comes with a "scenarios.epa" database, which includes the Generic Scenario Operations available in the assessment. Periodically, EPA may distribute an updated database. To update your Generic Scenarios database, save the new "scenarios.epa" database to your hard drive, click on *File/Replace Generic Scenario Database*, and select the new "scenarios.epa" file.

# Viewing an Assessment's Revision History

You can save changes to an assessment without updating the "Date" field in the General tab. Each time you open an assessment and close it (with or without saving), the date/time of the ChemSTEER database file is updated. As a result, it may often be difficult to determine WHEN a particular assessment was last modified and saved.

To view the revision history of the current assessment (i.e., the open assessment in ChemSTEER), go to the *File* menu and click *Revision History*. This will activate the *Display Revision History* 

of the Assessment screen, which contains a table of records for each time the current assessment was saved. Each record contains the following information, as recorded at the time the assessment was saved:

- Saved On contains the date and time of the save (the save records are ordered by descending date/time);
- EPA ID Assessment Identifier from the General tab;
- CBI CBI indicator (Yes/No) from the General tab;
- Type Assessment Type from the General tab;
- Status from the General tab; and
- Fiscal Year from the General tab.

The <u>General Information Tab</u> topic contains a more detailed description for each of the identifying fields listed above.

Go to <u>Saving Your Assessment</u> for more information on how to save your assessment.

# Deleting an Assessment from the Database

You may select *File/Delete Assessment* to delete a previously saved assessment from a ChemSTEER database. ChemSTEER will display a navigation window for you to choose the database in which the assessment to be deleted is saved. Select the database and click *OK*.

If the database file contains only one Assessment record, ChemSTEER will delete that assessment automatically.

If the existing database file contains more than one Assessment record, a table of Assessment records will appear that includes six fields in the record: Type, Fiscal Year, Identifier, Consolidated Case, Date, and Status. You may click on any of these fields or on the gray rectangle to the left of the 'Type' field in the row of the Assessment record that you wish to delete. This will cause an arrow to appear in the gray rectangle in the row of Assessment record that you wish to delete. Once this arrow is in the row of Assessment record that you wish to delete button will cause that assessment to be deleted from the database.

You may also use the *Search* button to filter available assessments by one or more of the following parameters: Assessment ID, Assessment Type, Assessment Status, or Date Range. If you wish change your selection criteria, you can delete entered text from the Assessment ID and Date Range text boxes and hit the reset button(s) to clear the Assessment Type and/or Assessment Status drop-down box(es).

NOTE: You may not delete an assessment that is currently opened in ChemSTEER. If you attempt to delete an open assessment, ChemSTEER will display a warning message asking you to first close the open assessment. To close an assessment, choose *File/Close Assessment*.

# Import/Viewing CRSS Report

These options are for internal EPA use.

# Run Models (Advanced Users)

This menu option runs the Direct Model Access (for Advanced Users).

# **EDIT**

# Cutting, Copying, and Pasting

These features work similarly to the corresponding features in other Windows-based programs.

# **PREFERENCES**

# Setting Your Preference for the Default Database

You may click on the *Preferences* menu and select *Default Database* to view and change your default ChemSTEER database file. This default file will be the first file that ChemSTEER will use when using the *File/Open Assessment* and *File/Save Assessment* options from the *Windows* menu. To change the default file, you may click on the Browse button and use the navigation window that appears to select a ChemSTEER database file.

# Vapor Model Activation

You may click on the *Preferences* menu and select *Vapor Model Activation* to view or change the default adjusted vapor pressure range that is used to activate vapor models in subsequent new assessments. Each assessment will have its own, possibly unique, adjusted vapor pressure range. For any new assessment, the adjusted vapor pressure range in the *Preferences/Vapor Model Activation* menu item is the default for the adjusted vapor pressure range on the *Operation Parameters* tab, *Shared Parameters/Factors* subtab.

Following this initial defaulting, the adjusted vapor pressure range for the current assessment can only be changed on the *Shared Parameters/Factors* subtab. The adjusted vapor pressure range determines whether or not ChemSTEER selects vapor generation release and mass balance inhalation models as defaults in the assessment for many of the release sources/inhalation exposure activities for liquids. By changing the value(s) of the adjusted vapor pressure range (AVPlow and/or AVPhigh), you change when ChemSTEER will select the vapor generation release and mass balance inhalation models as defaults for the liquid release sources/inhalation exposure activities.

When a new assessment is created, its initial adjusted vapor pressure range (AVPlow and AVPhigh) is based on the adjusted vapor pressure range default for that workstation on which ChemSTEER is being run. A workstation's adjusted vapor pressure range can be changed by using the *Preferences/Vapor Model Activation* menu option. Changing the default adjusted vapor pressure range on the *Preferences/Vapor Model Activation* menu option only affects the default for that workstation.

The workstation's default adjusted vapor pressure range is set to the ChemSTEER default values when ChemSTEER is installed. It is generally recommended that the following settings be made:

AVPlow = 0.001 torr and AVPhigh = 35 torr.

These are the default values for ChemSTEER. Clicking the *Restore Defaults* button resets AVPlow and AVPhigh to these ChemSTEER default values.

ChemSTEER calculates several adjusted vapor pressures for each operation. These adjusted vapor pressures (AVPrm, AVPprod) may be viewed on the *Operation Parameters* tab, *Shared Parameters/Factors* subtab. ChemSTEER selects the calculated adjusted vapor pressure that is appropriate for each liquid release source/inhalation exposure activity and compares the AVP to the adjusted vapor pressure range in the *Shared Parameters/Factors* subtab.

If the AVP for the source/activity is <u>within</u> the adjusted vapor pressure range shown in the *Shared Parameters/Factors* subtab, then ChemSTEER will select the appropriate vapor generation release and mass balance inhalation models as defaults for the source/activity.

If the AVP for the source/activity is <u>outside</u> of the adjusted vapor pressure range shown in the *Shared Parameters/Factors* subtab, then ChemSTEER will not select any of the vapor generation release or mass balance inhalation models as defaults for the source/activity. It is recommended that other vapor generation and inhalation methods (e.g., monitoring data for the assessed chemical or an appropriate surrogate chemical) be used when adjusted vapor pressure is below 0.001 torr or above 35 torr.

# Specifying CRSS Database

You may click on the *Preferences* menu and select *Specify CRSS Database* to view and change your default CRSS database file. Note that this is for internal EPA use.

# **Reports**

# Generating and Viewing Summary Reports

Go to the Reports menu or tab to view and print or export a copy of the EPA-formatted *Initial Review Engineering Report (IRER)* and/or *Contact Report* from the working assessment.

The IRER is a specially formatted EPA report for internal use for summarizing estimates of workplace releases and exposures in a particular assessment. See the <u>IRER Format Details</u> section for more information.

The Contact Report summarizes the information obtained via an external contact. See the <u>Contact Report Format Details</u> section for more information.

Clicking on the *Reports* menu or tab and selecting *View IRER Report, View Contact Report, or View Combined IRER & Contact Report* will display the report in a view window from which you may print the report. You may also export the report directly into \*.txt, \*.pdf, or \*.rtf formats to a choice of destinations (e.g., disk) using the Save IRER Report, Save Contact Report, or Save Combined IRER & Contact Report options.

To view various pages of the report, click on the appropriate arrow icons on the menu bar of the view window.

To print the report, click on the printer-shaped icon on the menu bar of the view window.

To export the report, click on the envelope-shaped icon on the menu bar of the view window.

**NOTE:** When you attempt to export an IRER without completing the *Occupational Exposure Rating & the Consumer Use* in the *Physical State and Misc CRSS Info, Other Uses, Occupational Exposure Rating, and Consumer Use* input screen of the <u>Optional Information Tab</u>, ChemSTEER will display a warning message. You may click *Yes* to continue with the export without the exposure rating or the consumer use. Click *No* to cancel the export.

ChemSTEER contains several *Basis* text boxes located throughout the assessment in order for you to provide additional information on the particular input values and general assumptions used in the assessment. You are strongly encouraged to use these Basis boxes. Note: any carriage return entered within these boxes will appear as a "|" within the text when an existing assessment is opened and viewed within ChemSTEER. These carriage returns "|" will also appear in the reports generated by ChemSTEER.

The *IRER* and *Contact Report* use the database fields from the currently selected assessment within ChemSTEER. You are required to save the current assessment before running reports for new assessments or modified assessments (including re-running models). You must also have at least one operation in order for saved data to be displayed in the IRER report. See the User Guide topics, <u>IRER</u> Format Details and <u>Contact Report Format Details</u>, for more specific information about these reports.

## Generating or Exporting Assessment Reports Before All Models Are Run

If you have sources/activities included in your assessment and you have either never run the associated release or exposure models or have made changes to the settings or parameter values used by any of the selected models, you will receive a warning message when you attempt to generate or export the assessment, asking you to save your assessment first (see <u>Saving Your Assessment</u>).

# **IRER Format Details**

The *Initial Review Engineering Report (IRER)* is a specially formatted EPA report for internal use in summarizing estimates of workplace releases and exposures in a particular assessment.

## **Summaries of Releases and Exposures**

Release and exposure estimates for each source/activity are listed <u>separately</u> in the IRER. This includes any estimate for which two outputs were enabled – each output is listed as a separate release in the IRER. Be sure to read the <u>Calculating Two Sets of Results from a Single Model</u> topic for additional information.

## **Combined Releases**

Releases are listed individually; however, one special feature in the IRER should be noted. Until the *Combining Releases and Combining Exposures* functions are completed in a future version of ChemSTEER, the IRER <u>combines releases to all environmental media together</u> for each operation into a "Release Total" that appears after the itemized list of operation releases.

Releases are only combined within an operation if all of the release models have been executed successfully (i.e., all releases have days of release calculated to be greater than zero).

The "Release Total" is calculated by adding together all releases from all sites over all days. Within a release, ChemSTEER will use the greater value from either the Output 1 or Output 2 result for the Release Total.

Hint: it is often helpful to describe any coinciding releases to the extent possible within each itemized release, as shown in the example below. Go to the <u>Estimating Chemical Releases Tab</u> topic to read more about the *Introductory Notes for the Release Summary* input text.

## **Combined Exposures**

Exposures are not combined as a default. Each activity's exposure estimate is listed separately in the IRER.

# **The IRER Format**

A listing of the ChemSTEER fields used to populate the IRER is shown below (items or values taken from specific fields in ChemSTEER are denoted in italics):

INITIAL REVIEW ENGINEERING REPORT

CBI: [General tab, CBI Yes/No]

[General tab, Assessment Type or General tab, Assessment Type, Other or Other New Chem text][General tab, Fiscal Year]-[General tab, Identifier][General tab, Consolidated Case text]

[General tab, Status or General tab, Status, Other text] [General tab, Date]

ENGINEER: [General tab, Name (Assessors Column 1)] \ [General tab, Name (Assessors Column 2)]

PV (kg/yr): [Chemicals tab, Total Assessed Production Volume (PV)]

(PV is an integer if >= 1, else in scientific notation with one digit following the decimal point)

{If the Assessment Type = LVE or LVEMOD and the Submission PV is not binding and not 10,000 kg/yr on the Optional Information tab – Special LVE Considerations, ChemSTEER will display the Submission PV from the Special LVE Considerations and note the assessed PV from the Chemicals tab}

[Binding PV (if checked on the Optional Information tab – Special LVE Considerations), Import Only (if the Type of Notice on the Chemical tab is Import, but not Manufacturing), YX (if Exposure-Based = Yes on the Optional Information tab – Exposure-Based Criteria), NX (if
Exposure-Based = No on the Optional Information tab – Exposure-Based Criteria and the PV > 100,000 kg/yr, C.O.S (if checked on the Optional Information tab – Special LVE Considerations), P2REC (if checked on the Optional Information tab - Pollution Prevention Considerations)]

Revision Notes/Assessment Overview: [General tab, Revision Notes/Assessment] {appears only if General tab, Revision Notes/Assessment Overview field contains text}

SUBMITTER: [General tab, Company Name]

USE: [Chemical tab, General Description of End Use(s)]

OTHER USES: [Optional Information tab, Misc CRSS Info, Other Uses, Occupational Exposure Rating, and Consumer Use combo box (i.e., drop-down list), Other Uses]

MSDS: [Optional Information tab, MSDS/Label/Exposure Limits combo box, MSDS Requirements subtab, MSDS Included Yes/No]

Label: [Optional Information tab, MSDS/Label/Exposure Limits combo box, MSDS Requirements subtab, Label Included Yes/No]

{The following items appear only if the MSDS Included = Yes and/or if the Label Included = Yes on the Optional Information tab – MSDS/Label/Exposure Limits}

Gen Eqpt: [Optional Information tab, MSDS/Label/Exposure Limits combo box, MSDS Requirements subtab, General Equipment]

Respirator: [Optional Information tab, MSDS/Label/Exposure Limits combo box, MSDS Requirements subtab, Respirator]

Health Effects: [Optional Information tab, MSDS/Label/Exposure Limits combo box, MSDS Requirements subtab, Health Effects]

LVE PPE: [Optional Information tab, MSDS/Label/Exposure Limits combo box, LVE PPE subtab, LVE PPE] {Only applicable if the Assessment Type on the General tab is LVE or LVEMOD}

TLV/PEL: [Optional Information tab, MSDS/Label/Exposure Limits combo box, Exposure Limits subtab, Material] [Optional Information tab, MSDS/Label/Exposure Limits combo box, Exposure Limits subtab, Concentration] [Optional Information tab, MSDS/Label/Exposure Limits combo box, Exposure Limits subtab, Exposure Limit] [Optional Information tab, MSDS/Label/Exposure Limits combo box, Exposure Limits subtab, Exposure Limit] [Optional Information tab, MSDS/Label/Exposure Limits combo box, Exposure Limits subtab, Reference] [Optional Information tab, MSDS/Label/Exposure Limits combo box, Exposure Limits subtab, Reference] [Optional Information tab, MSDS/Label/Exposure Limits combo box, Exposure Limits subtab, Reference] [Optional Information tab, MSDS/Label/Exposure Limits combo box, Exposure Limits subtab, Reference] [Optional Information tab, MSDS/Label/Exposure Limits combo box, Exposure Limits subtab, Reference] [Optional Information tab, MSDS/Label/Exposure Limits combo box, Exposure Limits subtab, Reference] [Optional Information tab, MSDS/Label/Exposure Limits combo box, Exposure Limits subtab, Type of Material]

{Note: the TLV/PEL label appears once only if exposure limit data is available. Exposure limit data repeats for multiple chemicals.}

CRSS: [Optional Information tab, Misc CRSS Info, Other Uses, Occupational Exposure Rating, and Consumer Use combo box, CRSS Date]

Chemical Name: [Chemical tab, Chemical Name] {will not appear if Chemical Name is blank, but text is entered in Chemical Category}

Chemical Category: [Chemical tab, Chemical Category] {will not appear if Chemical Category is blank}

S-H2O: [Chemical tab, Solubility or Dispersible or Reacts] g/L @ [Chemical tab, Solubility Temperature]

VP: [Chemical tab, Vapor Pressure (VPchem)] torr @ [Chemical tab, Vapor Pressure Temperature] (scientific notation with one digit following the decimal point)

MW: [Chemical tab, Molecular Weight (MW)] [Chemical tab, %<500 ] %<500 [Chemical tab, %<1000 ] %<1000

Physical State and Misc CRSS Info:

[Optional Information tab, Physical State and Misc CRSS Info, Other Uses, Occupational Exposure Rating, and Consumer Use combo box, Phys State and Misc CRSS Info]

Consumer Use: [Optional Information tab, Other Uses, Occupational Exposure Rating, and Consumer Use combo box, Consumer Use Yes/No]

SAT (concerns): [Optional Information tab, SAT Data combo box, SAT Date]

Related cases and Misc SAT Info: [Optional Information tab, SAT Data combo box, Related Cases and Misc SAT Info] {only appears when text is entered}

Migration to groundwater: [Optional Information tab, SAT Data combo box, Migration to Groundwater] [Optional Information tab, SAT Data combo box, Other Migration to Groundwater Description]

PBT rating: P[Optional Information tab, SAT Data combo box, P Rating] B[Optional Information tab, SAT Data combo box, B Rating] T[Optional Information tab, SAT Data combo box, T Rating], [Optional Information tab, SAT Data combo box, PBT Additional Info]

Health: [Optional Information tab, SAT Data combo box, Health Rating] [{each of the following when checked Yes: Dermal, Drinking Water, Inhalation, Not Required, Other, Other Description XB testing required, XB testing text]

Eco: [Optional Information tab, SAT Data combo box, Eco Rating] [{each of the following when checked Yes: Water, Water text, Air, Landfill, Not Required, Other, Other Description XB testing required, XB testing text]

OCCUPATIONAL EXPOSURE RATING: [Optional Information tab, Misc CRSS Info, Other Uses, Occupational Exposure Rating, and Consumer Use combo box, Occupational Exposure Rating]

### NOTES & KEY ASSUMPTIONS:

[Optional Information tab, Notes & Key Assumptions combo box]

### POLLUTION PREVENTION CONSIDERATIONS:

[Optional Information tab, Pollution Prevention Considerations combo box, Optional P2 Information from the submission]

P2 Rec: [Optional Information tab, Pollution Prevention Considerations combo box, P2REC] {appears only when the P2REC box is checked}

EXPOSURE-BASED REVIEW: [Optional Information tab, Exposure-Based Criteria combo box, Exposure Based Yes/No] [Optional Information tab, Exposure-Based Criteria combo box, Number of criteria met] criteria met {appears only if Exposure-Based = Yes or No (not blank) in the Optional Information tab – Exposure-Based Criteria}

{The following list appears only if Exposure-Based = Yes in the Optional Information tab – Exposure-Based Criteria}

- # of workers exposed: [Optional Information tab, Exposure-Based Criteria combo box, Number of Workers Exposed] >1000? [Optional Information tab, Exposure-Based Criteria combo box, Number of Workers Criteria Met Yes/No]
- >100 workers with >10 mg/day inhalation exposure: [Optional Information tab, Exposure-Based Criteria combo box, >100 workers with >10 mg/day inhalation exposure Yes/No]
- 3) (a) >100 workers with 1-10 mg/day inh. exp. & >100 days/yr: [Optional Information tab, Exposure-Based Criteria combo box, >100 workers with 1-10 mg/day inh. exp. & >100 days/yr Yes/No]

(b) Routine Dermal Cont: >250 workers & >100 days/yr: [Optional Information tab, Exposure-Based Criteria combo box, Routine Dermal Cont: >250 workers & >100 days/yr Yes/No]

Basis: [Optional Information tab, Exposure-Based Criteria combo box, Basis]

page break \_

INITIAL REVIEW ENGINEERING REPORT

CBI: [General tab, CBI Yes/No]

[General tab, Assessment Type or General tab, Assessment Type, Other or Other New Chem text][General tab, Fiscal Year]-[General tab, Identifier][General tab, Consolidated Case text]

{Note: This page repeats for each operation}

[Operations tab, Operation Name]

Number of Sites/Location: [Operation Parameters tab, Mass Balance Parameters subtab, Number of Sites]

[Operation Parameters tab, Site Information subtab, Facility Name] [Operation Parameters tab, Site Information subtab, City] [Operation Parameters tab, Site Information subtab, State] [Operation Parameters tab, Site Information subtab, Zip]

Days/yr: [Operation Parameters tab, Mass Balance Parameters subtab, Operating Days per Year]

Basis: [Operation Parameters tab, Mass Balance Parameters subtab, Basis Box]

Process Description: [Operations tab, Description subtab, Process Description]

ENVIRONMENTAL RELEASES ESTIMATE SUMMARY

[Releases tab, Introductory Notes for the Release Summary text]

{The following repeats for each release source within the operation. Media are ordered within the operation in the same top left to bottom right order as shown in the Update Release Media Output Specifications screen (Water through Other):}

[Releases tab, Media of Release Button, Media]:

[Output Characterization]: [Daily Release Rate (scientific notation with one digit following the decimal point)] kg/site-day over [Days of Release] days/yr from [NS] site(s) or [Annual Release Rate Site] kg/site-yr from [NS] site(s) or [Annual Release Rate] kg/yr-all sites

[Output Characterization] {this second set of results appears only if two outputs are enabled}: [Daily Release Rate (scientific notation with one digit following the decimal point)] kg/site-day over [Days of Release] days/yr from [NS] site(s) or [Annual Site Release Rate Site] kg/site-yr from [NS] site(s) or [Annual Release Rate] kg/yr-all sites

from: [Releases tab, Source]

to: [Releases tab, Modify Media of Release screen, To (NPDES number if appropriate)]

basis: [Releases tab, View/Update Release Model Information screen]

RELEASE TOTAL: [Sum of Annual Release Rate for all sources in the operation (scientific notation with one digit following the decimal point)] kg/yr – all sites

[Releases tab, Additional Notes for the Release Summary text]

### OCCUPATIONAL EXPOSURES ESTIMATE SUMMARY

Tot. # of workers exposed via assessed routes: [Exposures tab, Update Operation Total Number of Workers Exposed button, Operation total number of workers estimated]

Basis: [Exposures tab, Update Operation Total Number of Workers Exposed button, Basis]

### Inhalation:

[Exposures tab, Inhalation Model Input Parameters subtab, Introductory Notes for the Inhalation Summary]

{The following repeats for each inhalation model within the operation (if applicable):}

Exposure to [Exposures tab, Inhalation Model Input Parameters, Chemical State] ([volatile] or [non-volatile]) {If the chemical is Mist or Aerosol}

{For respirator class selection [Exposure tab, Respirator Class and Monitoring Review subtab] (logic below), the chemical is assumed to be volatile if AVPprod > AVPlow for product-related activities or if AVPrm > AVPlow for any other activity}

(Class I) {If the chemical state is Particulate, or if the AVP associated with the activity is non-volatile and the chemical state is Mist or Aerosol}

(Class II) {If the chemical state is Vapor}

(Class III) {If the AVP associated with the activity is volatile and the chemical state is Mist or Aerosol}

[Exposures tab, Inhalation Model Input Parameters, Characterization]: [Exposures tab, Activity Exposure Estimates, Inhalation Potential Dose Rate] mg/day over [Exposures tab, Inhalation Model Input Parameters, Exposure Days] days/yr

[Exposures tab, Inhalation Model Input Parameters, Characterization]: [Exposures tab, Activity Exposure Estimates, Inhalation Potential Dose Rate] mg/day over [Exposures tab, Inhalation Model Input Parameters, Exposure Days] days/yr {this second set of results appears only if two outputs are enabled}

Number of workers (all sites) with inhalation exposure: [Exposures tab, Inhalation Model Input Parameters, NWexp x NS] {maximum NWexp x NS if two outputs are enabled}

{One of the following texts is displayed, based on the appropriate respirator class [Exposure tab, Respirator Class and Monitoring Review subtab]: "NOTE: The respirator class is ["I. Particulate (including solid or liquid droplets)"; "II. Gas/vapor (all substances in the gas form)"; or "III. Combination Gas/Vapor and Particulate (gas and liquid/solid physical forms are both present)"]."}

basis: [Exposures tab, Exposure Activity]; [Exposures tab, Inhalation Model Input Parameters, Basis]

INHALATION MONITORING DATA REVIEW [Exposure tab, Respirator Class and Monitoring Review subtab]

1) Uncertainty (estimate based on model, regulatory limit or data not specific to that industry)

Yes/No

(Yes/No determined based on the Uncertainty checkbox on the View/Update Exposure Model Information screen of the Exposures tab)

2) (a) Exposure level > 1 mg/day Yes/No

(Yes if Output 2 is > 1 mg/day for two outputs or if a single output is > 1 mg/day, else No)

OR

(b) Hazard Rating for health of 2 or greater? [Optional Information tab, SAT Data combo box, Health Rating] Yes/No

(Yes if [Optional Information tab, SAT Data combo box, Health Rating] = 2, 2-3, or 3, else No (or null if Health Rating is null))

Inhalation Monitoring Data Desired? Yes (both criteria met)/No

(Yes if 1) is Yes and 2(a) or 2(b) is Yes, else No (or null if Health Rating is null))

Dermal:

[Exposures tab, Dermal Model Input Parameters subtab, Introductory Notes for the Dermal Summary]

{The following repeats for each dermal model within the operation:}

Exposure to [Exposures tab, Dermal Model Input Parameters, Chemical State] at [Exposures tab, Dermal Input Parameters, Weight Fraction x 100] % concentration

[Exposures tab, Dermal Model Input Parameters, Characterization]: [Exposures tab, Activity Exposure Estimates, Dermal Exposure Dose Rate] mg/day over [Exposures tab, Dermal Model Input Parameters, Exposure Days] days/yr

[Exposures tab, Dermal Model Input Parameters, Characterization]: [Exposures tab, Activity Exposure Estimates, Dermal Exposure Dose Rate] mg/day over [Exposures tab, Dermal Model Input Parameters, Exposure Days] days/yr {this second set of results appears only if two outputs are enabled}

Number of workers (all sites) with dermal exposure: [Exposures tab, Dermal Model Input Parameters, NWexp x NS] {maximum NWexp x NS if two outputs are enabled}

basis: [Exposures tab, Exposure Activity]; [Exposures tab, Dermal Model Input Parameters, Basis]

### **Contact Report Format Details**

The Contact Report summarizes the information obtained from an external contact.

There are two separate formats for the Contact Report, depending upon whether the report contains confidential business information (CBI) or does not contain CBI.

A listing of the ChemSTEER fields used to populate each of the contact report types is shown below (information from fields in ChemSTEER are denoted in *italics*):

### **CBI Contact Report Format**

The following format is used if the CBI field shows *Yes* (i.e., contact report does contain TSCA CBI) in the *General* tab, *View/Update Contact Reports* window:

CBI: Yes

MEMORANDUM of TSCA CBI TELEPHONE CONVERSATION

CALL BY:	[General tab, View/Update Contact Reports window, Called By]
Organization:	[General tab, View/Update Contact Reports window, Called By Affiliation]
CALL TO:	[General tab, View/Update Contact Reports window, Call To]
Organization:	[General tab, View/Update Contact Reports window, Call To Affiliation]
Date:	[General tab, View/Update Contact Reports window, Call Date]
Time:	[General tab, View/Update Contact Reports window, Call Time]
Phone:	[General tab, View/Update Contact Reports window, Phone]

Concerning what TSCA CBI?

[General tab, Assessment Type or General tab, Assessment Type, Other, or Other New Chem text] [General tab, Fiscal Year]-[General tab, Identifier] [General tab, Consolidated Case text]

[General tab, View/Update Contact Reports window, Applicable Assessments]

Content

[General tab, View/Update Contact Reports window, Notes]

### Contact Report Format (Report does not contain TSCA CBI)

The following format is used if the CBI field shows No (i.e., contact report does not contain TSCA CBI) in the *General* tab, *View/Update Contact Reports* window:

CBI: No

MEMORANDUM of TELEPHONE CONVERSATION (Contains No TSCA CBI)

CALL BY: Organization:	[General tab, View/Update Contact Reports window, Called By] [General tab, View/Update Contact Reports window, Called By Affiliation]
CALL TO: Organization:	[General tab, View/Update Contact Reports window, Call To] [General tab, View/Update Contact Reports window, Call To Affiliation]
Date:	[General tab, View/Update Contact Reports window, Call Date]
Time:	[General tab, View/Update Contact Reports window, Call Time]
Phone:	[General tab, View/Update Contact Reports window, Phone]

Concerning what?

[General tab, Assessment Type or General tab, Assessment Type, Other or Other New Chem text] [General tab, Fiscal Year]-[General tab, Identifier] [General tab, Consolidated Case text]

[General tab, View/Update Contact Reports window, Applicable Assessments]

Content [General tab, View/Update Contact Reports window, Notes]

# Guide to Using ChemSTEER Tabs

The following sections discuss the eight main tabs in ChemSTEER:

- 1. General Information Tab
- 2. <u>Chemical Properties Tab</u>
- 3. Operations Tab
- 4. Operations Parameters Tab
- 5. Estimating Chemical Releases Tab
- 6. Estimating Chemical Exposures Tab
- 7. Optional Information Tab
- 8. <u>Reports Tab</u>

# **GENERAL INFORMATION TAB**

This tab allows you to view and/or enter general information related to the ChemSTEER assessment, which includes assessment/case identifiers, status, the assessor(s) and other general information about the assessment. None of these fields is required in completing an assessment. However, ChemSTEER will not allow the four *identifying fields* to be identical when saving to a database containing more than one assessment.

### **Identifying Fields**

ChemSTEER differentiates each assessment in a database containing more than one assessment by the information in the four *Identifying Fields*:

- Assessment Type,
- Status,
- Fiscal Year, and
- Identifier.

To prevent storage of apparently duplicate assessments in one database file, ChemSTEER requires that information in one or more of the *Identifying Fields* be different for each assessment. When *Save* or *Save As* is used, ChemSTEER compares the *Identifying Fields* in the current assessment with the *Identifying Fields* of assessments already in the database (Save) or in the destination database (Save As) to ensure that no assessments in a database have identical identifying fields. These key identifying fields and the assessment date will be displayed when you open a database containing multiple assessments.

ChemSTEER displays these four identifying fields, along with the dates/times the assessment was saved, when <u>Viewing an Assessment's Revision History</u>.

Assessment Type: Type of assessment. (One of the four identifying fields.)

Drop down list (most of these are typically used by EPA for its reviews of new and existing chemicals):

- C (Correction),
- LOREX (low release and exposure exemption),
- LOREXMOD (low release and exposure exemption modification),
- LVE (low volume exemption),
- LVEMOD (low volume exemption modification),
- PMN (premanufacture notice),
- SNUN (significant new use notification)
- TME (test marketing exemption),
- I (enforcement),
- Other New Chem (text box appears for Other New Chem),
- Existing Chemical,
- OECD-SIDS (Organisation for Economic Co-Operation and Development Screening Information Dataset),
- RM1 (preliminary risk management assessment),
- RM2 (detailed risk management assessment (post-RM1), and
- Other (text box appears for Other).

NOTE: To find out more about OPPT's assessments, go to EPA's web site and search on the assessment type.

**Status:** Status of the report. (One of the four identifying fields.) Drop down list (most of these are typically used by EPA for its reviews of new chemicals):

- Contractor Draft,
- CEB Staff Draft,
- Focus Ready Draft,
- Standard Review Draft,
- Post-Focus Draft Revision 1,
- Post-Focus Draft Revision 2,
- Post-Focus Draft Revision 3,
- Post-Focus Draft Revision 4,
- Post-Focus Draft Revision 5, and
- Other (text box appears for Other).

Fiscal Year: Fiscal year field. (One of the four identifying fields.)

The fiscal year is for entering a two digit numerical code. For example, fiscal year 2004 is from 1 October 2003 through 30 September 2004, thus the fiscal year code for 2004 is '04'.

**Assessment Identifier:** Identifying number or text for the assessment. (One of the four identifying fields.)

If the Assessment Type is one of the "new chemicals" types, which include: *C*, *LOREX*, *LOREXMOD*, *LVE*, *LVEMOD*, *PMN*, *SNUN*, *TME*, *I*, and *Other New Chem*, then the Assessment Identifier is limited to a four digit numerical code.

For any other Assessment Type, the Assessment Identifier is a text field.

### **Remaining Fields on the General Tab**

The following is a list of fields and buttons and the descriptions of each:

**Consolidated Case:** Designates whether the assessment contains a group of more than one chemical. Yes or No checkbox. If *Yes*, a text box appears.

**Date:** Date of completion corresponding to the *Status*. ChemSTEER dates the assessment when first created.

NOTE: Upon clicking *Save* or *Save As*, ChemSTEER first checks to see if the date matches today's date. If not, a message appears asking you if you wish to change the date. Clicking *Yes* causes ChemSTEER to update the date to today's date.

**CBI:** A check box to indicate if the assessment contains TSCA Confidential Business Information. An "x" in the box indicates *Yes*.

*Number of Contact Reports:* Number of phone logs. ChemSTEER keeps track of the number of phone logs entered in the assessment. This is displayed in *General* tab.

Name: Name of the assessor Affiliation: Affiliation of the assessor Phone: Phone number of the assessor Email: Email of the assessor

Company Name: company name Street Address: company address City: company city State: company state Zip: company zip code

Revision Notes/Assessment Overview: Brief notes about the assessment

**Update General Information button:** Button to display the Update General Information data entry screen.

*View/Update Contact Report button:* Button to display the View/Update Contact Reports screen.

If you previously contacted the person and saved the contact report in the assessment, you can quickly transfer the contact information to the new report by selecting the earlier report and clicking Add/Copy in the View/Update Contact Reports screen. You may then modify any of the contact information as appropriate for new contact report.

This information can be printed or saved to a text file of a Contact Report (see <u>Contact Report</u> <u>Format Details</u>).

Update Revision Notes/Assessment Overview button: Button to display a text box for assessment notes and/or overview.

# **CHEMICAL PROPERTIES TAB**

You can view and/or enter information about the chemical to be assessed using the Chemical tab in ChemSTEER.

Many of the fields shown are for chemical parameters that are commonly used by EPA in completing assessments. Chemical identification and use fields are for identification and informational purposes. These fields include chemical identification information including: chemical name and category; CAS number; molecular formula; and a description of intended use(s) of the chemical (e.g., chemical function and end use application, such as surfactant in industrial laundry detergent).

The fields labeled in RED are required inputs for many of ChemSTEER's calculations of mass balance, releases and worker exposures. Volume parameters are used extensively in the mass balance and container parameters calculations and in generating release- and exposure-related estimates. Volume parameters include import and domestic production volumes (or volumes to be assessed).

Physical/chemical properties are parameters that are also commonly used in several of the ChemSTEER models (e.g., vapor pressure, molecular weight, density).

The Type of Notice designator is used by EPA in distinguishing between reviews for chemicals that are manufactured domestically (Manufacturing) and/or imported to the U.S. for further processing and use (Import).

Click on *the Update Chemical Information* button at the bottom of the tab to revise fields shown on the tab.

Click on the *View/Update Exposure Limits* button to see a readily available <u>List of OSHA PELS and</u> <u>NIOSH RELs</u> obtained for several chemical substances.

NOTE: Be aware that changing certain parameters on this tab will affect the mass balance calculations, container-related calculations, and release and exposure model estimates. Be sure to read about ChemSTEER's <u>Hierarchy of ChemSTEER Operations</u>, <u>Activities</u>, and <u>Models</u>.

# **OPERATIONS TAB**

In ChemSTEER, the term "Operation" refers to a workplace or set of "homogeneous" workplaces with essentially the same (or similar) processes, equipment, chemical throughputs, procedures, and worker populations, such that estimates of releases and exposures to the chemical being assessed can be assumed to be essentially the same for all of the workplaces, if more than one, in the set. If workplaces differ in some aspects that could result in significantly different estimates of releases and exposures, you should assess these workplaces as two or more separate operations.

There are typically three types of operations in ChemSTEER: Manufacturing, Processing, and Use. In ChemSTEER, the term "Manufacturing" is generally intended to represent an operation in which the chemical being assessed is created or formed in a reaction. The term "Processing" is generally intended to represent an operation in which the chemical being assessed is not created or formed and in which the chemical being assessed is not destroyed or transformed in a chemical reaction, or otherwise becomes essentially unavailable for further release or exposure. Formulation and repackaging operations would usually be considered to be types of Processing operations. The term "Use" is generally intended to represent an operation in which the chemical being assessed destroyed or transformed in a chemical reaction, or otherwise becomes essentially unavailable for further release or exposure.

You can use the *Operations* tab to view and/or select operations to assess and to view and/or enter information about each operation's process description, relationships to other operations, the physical state(s) of the chemical or the mixture containing the chemical, the release source/exposure activities, and site-specific location and associated information.

# Define/Select Operations to be Assessed

You should first click the "Add/Update Operations" button at the top of the screen, which you can use to add or delete operations to be assessed. You may add the same operation more than once. For example, if you wish to assess two different formulation operations, you can add User-defined Processing twice, and ChemSTEER will label the second addition as User-defined Processing 2.

NOTE: You must select at least one operation to access the ChemSTEER release and exposure models.

The Add/Update Operations screen has three tabs with different options for adding operations:

- User-defined Operations
- Generic Scenario Operations
- Import Operation

These three options are discussed in the subsections below.

### **User-defined Operations**

The three available User-defined operations (User-defined Manufacturing, User-defined Processing, and User-defined Use) are for use when none of the generic scenario operations are appropriate for assessing a workplace of interest. Industry-specific operations have a predetermined set of default values to define some key parameters used to estimate mass balances, releases, and

exposures. Some industry-specific operations have associated industry-specific source/activities and models, while others preselect standard default source/activities from the available list in ChemSTEER. User-defined operations rely upon you to provide the source/activities, mass balance, and many other parameter values.

NOTE: It is not recommended that you attempt to utilize the User-Defined Manufacturing operation for neither a processing or use scenario, nor that you use the User-Defined Use operation for either a processing or manufacturing scenario. These user-defined operations were specifically designed to be used for their associated scenarios and have options specific to each type of operation.

### **Generic Scenario Operations**

There are three industry-specific operations that have previously been hard-coded into ChemSTEER, which include:

- Automobile Original Equipment Manufacture (OEM) Spray Coating,
- <u>Electroplating Bath Additive Use, and</u>
- <u>Recirculating Water-Cooling Tower Additive Use</u>.

These scenarios were created prior to the September 30, 2013 version of ChemSTEER and have specific logic and all possible default/non-default values programmed into the scenario. Since the September 30, 2013 version, ChemSTEER allows EPA to save simple generic scenarios to the list, which provide templates for assessment and include the most conservative default values from the Generic Scenarios, such as the Use of Photoresist in Semiconductor Manufacturing. These versions have specific source/activities added, with default parameters included. Parameters can be modified based on additional information from the submitter. You should review the Help files included for each scenario to determine the most appropriate default estimates for your assessment.

The Generic Scenario operations are stored in a scenarios.epa database, for which EPA may distribute updates in the future (see <u>Replacing the Generic Scenario Database</u>).

# **Import Operations**

In some cases, you may want to complete an assessment similarly to an assessment you have previously completed. In this case, you can import one more operations from an older assessment into your current assessment.

To select an operation, first click the "select database" button and specify the database/assessment which has the operation(s) you are interested in. Double-click the operation, or select the operation and click "Add to list" This will import the operation into your current assessment.

ChemSTEER will import the operation, sources/activities, and release and exposure models into your assessment. Note that the relationship for this operation will be successive to any previously added operation, and the PVop for the imported operation will be set equal to the previous operation.

Note that since the PVop may have changed, you are required to manually update the mass balance parameters (Operation Parameters Tab  $\rightarrow$  Mass Balance Parameters Subtab) before running models.

# **Rename Default Operation Titles**

You can rename an operation to more accurately describe the operation. It is recommended that if you do rename an operation, that you maintain the original label for that operation, perhaps in parenthesis, after the new name (e.g., "Formulation of Paint Products (User-defined Processing) ). The original label can be helpful in reminding you what type of ChemSTEER operation you chose.

# Set the Order of Operations Within the Assessment

The operation "ordering" is consistent with their listing in the various tabs and screens in ChemSTEER and reports (i.e., from top to bottom). The default order of operations is the order in which you originally selected them in building the assessments. The order of operations is completely independent of the operation relationships. ChemSTEER passes appropriate variables from operation to operation (e.g., Yprod -> Yrm) based on the order of relationships set within the <u>Operations Tab  $\rightarrow$  Relationships Subtab</u>.

When an assessment contains more than one operation, you may change the order of operations in the *Update Operations* window by first clicking on the operation to be "moved" in the "Selected Operations" grid. The click *Move Up* and/or *Move Down*, as appropriate, to "move" that operation up or down within the assessment.

NOTE: Ordering operations on the *Operations* tab will have no affect on relationships specified on the *Relationships* tab. Setting the order on the *Operations* tab will only affect the order of operation display (top to bottom) on summary reports and on the Operations, Operation Parameters, Releases, and Exposures tabs.

If you reorder the operations, the following warning message will appear once you confirm by clicking *OK*:

"You have modified the display of operations, you should return to the *Relationships* tab to also modify the relationships (if appropriate)."

<u>Example:</u> You may determine, after completing an import only assessment, that manufacturing may be domestic and should be added to the assessment. You add manufacturing on the *Update Operations* tab. By default, ChemSTEER adds manufacturing as the last operation (since it was selected last). If appropriate, you may select manufacturing and use the *Move Up* button to place manufacturing as the first-listed operation. You <u>also</u> need to modify the relationships on the *Relationships* tab such that manufacturing has no proceeding operations and then specify the operations subsequent to manufacturing.

# **Removing Operations from the Assessment**

To remove an operation from the assessment, select the operation in the "Selected Operations" grid and click *Remove from list*. If you remove an operation from the assessment, you will receive the following message:

"Are you sure you want to remove the [name] operation from the assessment?

If you remove this operation from the assessment, all of the information associated with this operation will be removed from the assessment and you will need to reset all relationships in the assessment"

Simply click *Yes* to confirm the removal.

As stated in the warning, you should go to the <u>Operations Tab  $\rightarrow$  Relationships Subtab</u> and reverify the relationships for the operations remaining in the assessment.

# Working with the Operation Subtabs

The data and information contained in the subtabs in the lower half of the *Operation* tab are relevant to the Operation that is selected. To select an operation, click on the desired operation label in the list on the upper half of the Operation tab. The selected Operation is then highlighted. To update the data fields for any of the subtabs (Description, Relationships, Physical States, Source/Activities, and Site Information), click on the subtab label and then click on the *Update* button appropriate to the subtab. An *Update* window will appear and you can click on the data field and enter the appropriate information. Clicking the *OK* button at the bottom of the window will enter the new information into the assessment.

You must specify relationships (see <u>Operations Tab  $\rightarrow$  Relationships Subtab</u>) between more than one operation within an assessment, which enables certain default values and calculations to execute properly in ChemSTEER.

You must also select at least one Source/Activity that uses the model that you wish to use in order to access that model. Source/Activities may be viewed as access vehicles to allow you to use models. Refer to the <u>Release Sources and Exposure Activities</u> topic in this User Guide to determine which models are the defaults for each source/activity.

# Operations Tab → Relationships Subtab

In ChemSTEER, the term "Relationship" refers to how different workplaces are related as suppliers and customers. A customer's operation receiving the chemical being assessed from a supplier, whether pure or in a mixture with other chemicals, makes the customer's operation a *subsequent operation* to the supplier's operation. As a default, ChemSTEER assumes a simple serial relationship, with each operation on the list being the subsequent operation to the previous operation – in the order that they were selected for the assessment in the *Update Operations* screen of the *Operations* tab.

You must specify the relationship between multiple operations within an assessment, which enables certain default values and calculations to execute properly in ChemSTEER. For example, a manufacturer of a chemical in a solution (i.e., a *supplier* assessed via the *User-defined Manufacturing* operation) provides that solution to a formulator who blends the chemical solution into a new product (i.e., a *customer assessed* via the *User-defined Processing* operation). For this assessment, you should designate the User-defined Processing as a <u>subsequent</u> operation to User-defined Manufacturing. Then, ChemSTEER assumes that the weight fraction of the chemical in solution leaving the User-defined Manufacturing operation (Yprod) is equivalent to the weight fraction of the chemical in the solution entering the User-defined Processing (Yrm) as a default.

**NOTE:** If you modify a previously saved relationship, it is <u>highly recommended</u> that you reverify the default parameter values in the <u>Operations Parameters Tab</u>.

### Important Notes to Remember when Modifying the Default Relationships

An operation cannot be specified as a subsequent operation more than one time. For example, if you select Operation B as subsequent to Operation A and then select Operation B again as subsequent to another Operation C, ChemSTEER will designate the last relationship made (i.e., Operation B is subsequent to Operation C only) and will reassign the *Percent of PV* and *PVop* as discussed below.

To "move" an operation from the first position in the assessment, select that operation and verify that the box next to "This operation has no preceding operations" is <u>unchecked</u> in the *Update Operation Relationships* screen. That operation may then be added to the list of subsequent operations that follow another.

To "move" an operation to the first position in the assessment, you must first remove the operation from any list of subsequent operations in the assessment (by clicking each operation and viewing the list in the *Update Operation Relationships* screen for each). Next, select that operation (to be in the first position) and verify that the box next to "This operation has no preceding operations" is <u>checked</u> in the *Update Operation Relationships* screen. You may then add operations to the list of subsequent operations, as appropriate.

### The PVop and Percent of PV Parameters

Two important parameters in operation relationships are *PVop* and *Percent of PV*. Percent of PV represents the *PERCENT* of the *total assessed production volume (PV)* (entered on the *Chemicals* tab) that flows into or from an operation. For example, if a manufacturing operation (User-defined Manufacturing) produces all of the total assessed PV, then the *Percent of PV* for User-defined Manufacturing is 100 (100%). If there are two primary use operations (User-defined Use and User-defined Use 2) that are subsequent to the User-defined Manufacturing and three quarters is used by the first use operation and the remainder by the second use operation, then the *Percent of PV* for User-defined Use is 75 (75%) and the *Percent of PV* for User-defined Use 2 is 25 (25%).

*PVop* is the production volume (kg/yr) that is processed within each operation of the assessment. In other words, each operation contains a unique *PVop* that is less than or equal to the *total* assessed *PV*, where:

PVop (kg/yr) = (Percent of PV/100) x total assessed PV

You may change the values of *Percent of PV* or *PVop* for each subsequent operation. Typically, the following limitations would apply:

- The sum of PVops for all subsequent operations is equal to the PVop in the preceding operation; and
- The sum of Percent of PVs for all subsequent operations is equal to the Percent of PV in the preceding operation.

For example, if Operations M and N are subsequent to Operation L, which has a *Percent of PV* = 60 (60%) and a *PVop* of 60,000 kg/yr, then the *Percent of PV* for Operations M and N should add to 60 (60%), and their *PVops* should add to 60,000 kg/yr.

However, ChemSTEER <u>will allow</u> you to enter *PVops* and *Percent of PVs* for subsequent operations that are not equivalent to those of the preceding operation.

For example, in the scenario shown below, the subsequent operations' PVops are less than the preceding operation's PVop:



To create this relationship, the *Mfr*, *Use 1*, and *Use 2* operations were added to the assessment by clicking the Update Operations button on the Operations tab (see <u>Operations Tab</u>). The relationship shown above is established by designating both *Use 1* and *Use 2* as subsequent operations to *Mfr*. To do this, click on the Relationships subtab. Select *Mfr* in the upper box of the Operations tab and then click the *Update Relationships* button to view the *Update Operation Relationships* screen.

First, update the PVop for *Mfr* to be 75% PV (it defaults to 100% PV). You may already see *Use 1* in the list of subsequent operations in the lower portion of the screen (if it was added to the assessment right after *Mfr* was added). To establish the above relationship, be sure that both *Use 1* and *Use 2* are added to the *Subsequent Operations* list for the selected *Mfr* operation. Next, update each of the subsequent operations' PVops or Percent of PVs to be:

PVmfr = 20% PV; and PVuse1 = 30% PV

Clicking *OK* to return to the Relationships subtab. *Use 1* will display PVop = 20% PV and *Use 2* will display PVop = 30% PV.

In the scenario illustrated below, the subsequent operations' PVops exceed both the preceding operation's PVop, as well as the total assessed PV entered on the Chemicals tab:



Initially, the *Mfr* and *Use 1* operations were added to the assessment. Initial defaults for each of the PVops are:

PVmfr = 100% PV; and PVuse1 = 100% PV

When *Use 2* is added as a second, subsequent operation to Mfr, it is added with an initial PVuse2 = 0% PV.

You may then change the PVop for Use2 (PVuse2) to equal 30% PV in the *Update Operation Relationships* screen.

Clicking off the PVuse2 cell does not change the PVop or Percent of PV values (i.e., PVuse1 = 100% PV and PVuse2 = 30% PV).

Clicking *OK* to return to the Relationships subtab. Use 1 will display PVop = 100% PV and Use 2 will display PVop = 30% PV. Added together, these account for 130% of the total assessed PV.

ChemSTEER will allow the PVops for a set of subsequent operations to exceed <u>the total assessed</u> <u>PV</u> entered on the Chemical tab. For this reason, you should use caution when entering PVops and Percent of PVs in relationships to ensure that you do not exceed the assessment's total PV.

Entering PVops or Percent of PVs that are not equal to the preceding operation's PVop or Percent of PV allows you to model the following:

A subsequent operation that has a PVop that <u>exceeds</u> the preceding operation can account for <u>an import</u> of a portion of the total assessed PV at a point between the preceding and subsequent operations; and

A subsequent operation that has a PVop <u>that is less than</u> the preceding operation can illustrate <u>an export</u> of a portion of the total assessed PV at a point between the preceding and subsequent operations.

Operations Tab  $\rightarrow$  Description Subtab

The *Description* subtab allows the user to record NAICS Code, related description information, and process description for the operation. For industry-specific operations, default process descriptions are normally provided and are available for editing. Process descriptions, including physical form and concentration at the beginning and end of the operation, are particularly important in determining a complete set of sources/activities to assess.

# Operations Tab $\rightarrow$ Physical States Subtab

The Physical States subtab allows the user to record physical states for the operation. For industry-specific operations, default physical states may be provided, which are available for editing.

Future versions of ChemSTEER will use the physical state information input in this subtab to present a shorter list of more likely sources/activities to the user.

# Operations Tab → Sources/Activities Subtab

In ChemSTEER, the term *Source/Activity* refers to sources and activities in an operation that can/do/will cause environmental releases and/or worker exposures. Most Sources/Activities have one or more default models that ChemSTEER uses to estimate releases and exposures. Choosing appropriate Sources/Activities allow you to access the models to make these estimates.

Many industry-specific operations in ChemSTEER have preselected default Sources/Activities based on the sources and activities that are expected to occur in these operations. The user-defined operations require that you select the relevant Sources/Activities to assess.

Some Sources/Activities are specific to a particular industry (e.g., the Automotive Refinish Spray Coating Application source/activity), while other sources/activities are "broadly applicable" across many workplaces (e.g., the Loading Liquid Product into Drums or the Sampling Solid Raw Material sources/activities). The broadly applicable sources/activities available in ChemSTEER are only a subset of all possible sources and activities and cover those that are often overlooked or considered to be non-routine or insignificant.

When none of the other available Sources/Activities seem to cover a particular source/activity that you wish to assess, you may wish to choose from the Sources/Activities listed under the *Miscellaneous Sources/Activities* category, which allow you the greatest flexibility in using ChemSTEER to estimate releases and/or exposures (i.e., these miscellaneous Sources/Activities allow you to choose the most appropriate release/exposure methods and models to use in the calculations.

Each selected Source/Activity activates one or more equations that represent methods and models that will quantify the release and/or exposure estimate(s). You can read more about the default methods and models, as well as the most appropriate alternatives, for each of the Sources/Activities under the <u>Release Sources and Exposure Activities</u> section of the User Guide.

### Adding Sources/Activities to an Operation Assessment

When you update the Source/Activity list for an operation, clicking on the *Update* Sources/Activities button activates an *Update* window. At the top of the *Update* window is a list that initially shows the Source/Activity *Category* names. At the bottom of the *Update* window is a list of Sources/Activities that will be included and assessed for the selected operation.

Double-clicking on a particular Source/Activity Category name opens the list of available Sources/Activities relevant to the Category. You may either select the Source/Activity that you wish to add to the operation assessment by clicking on it in the upper list and then clicking on the *Add To List* button to add the Source/Activity to the list that will be assessed for the selected operation in ChemSTEER. Alternately, you may double-click on the Source/Activity that you wish to add to the operation assessment.

Sources/Activities are numbered in the order that they are added to the assessment. Currently, there is no functionality to the numbering, and these numbers are carried through the Release and Exposures tabs.

Note: you may include up to 20 sources/activities within each operation of the assessment.

### Automated Addition of Container Unloading and Cleaning Sources/Activities

In most cases wherever a container is unloaded, there are also empty container residues that are disposed or cleaned within the same operation. For this reason, ChemSTEER will automatically add the corresponding container cleaning source/activity when you add a container unloading source/activity and vice versa.

A summary of these corresponding container unloading and cleaning sources/activities is provided below:

Container Unloading Sources/Activities	Container Residue Disposal/Cleaning Sources/Activities		
Raw N	laterial		
Unloading Liquid Raw Material from Bottles	Cleaning Liquid Residuals from Bottles Used to Transport Raw Material		
Unloading Liquid Raw Material from Small Containers	Cleaning Liquid Residuals from Small Containers Used to Transport Raw Material		
Unloading Liquid Raw Material from Drums	Cleaning Liquid Residuals from Drums Used to Transport Raw Material		
Unloading Liquid Raw Material from Totes	Cleaning Liquid Residuals from Totes Used to Transport Raw Material		
Unloading Liquid Raw Material from Tank Trucks	Cleaning Liquid Residuals from Tank Trucks Used to Transport Raw Material		
Unloading Liquid Raw Material from Rail Cars	Cleaning Liquid Residuals from Rail Cars Used to Transport Raw Material		
Unloading Liquid Raw Material from Containers	Cleaning Liquid Residuals from Containers Used to Transport Raw Material		
Unloading Solid Raw Material from Transport Containers	Cleaning Solid/Powder Residuals from Containers Used to Transport Raw Material		
Product			
Unloading Liquid Product from Containers	Cleaning Liquid Residuals from Containers Used to Transport the Product		
Unloading Solid Product from Transport Containers	Cleaning Solid/Powder Residuals from Containers Used to Transport the Product		
User-Defined Material			
Unloading Liquid from Storage/Transport Containers (User-defined)	Cleaning Liquid Residuals from Storage/Transport Vessels (User-defined)		
Unloading Solids from Storage/Transport Containers (User-defined)	Cleaning Solid Residuals from Storage/Transport Vessels (User-defined)		

The automatic addition of these sources/activities will only occur if you do NOT already have the source/activity added for the operation. If you do not wish to include either the container unloading or cleaning source/activity, you may delete it from the operation at any time (see below).

### **Removing Sources/Activities from an Operation Assessment**

To remove a Source/Activity from the list of Sources/Activities that will be assessed in ChemSTEER (the lower list on the *Update* window), you may select the Source/Activity that you wish to remove from that list by clicking on it, then click the *Remove From List* button. A warning window will ask you to verify that you wish to remove that Source/Activity from the operation assessment. Simply click *Yes* to proceed.

### **Renaming Sources/Activities**

You may wish to rename a Source/Activity in order to denote it with a more appropriate or descriptive label. To rename a Source/Activity in the list of selected Sources/Activities to be assessed in

ChemSTEER (the lower list on the *Update* window), simply click on the Source/Activity and type the new name in the field.

### Specifying the Type of Source/Activity Assessment

In the list of selected Sources/Activities to be assessed in ChemSTEER (the lower list on the *Update* window) there are columns that determine whether ChemSTEER will assess releases and/or exposures for each of the selected Sources/Activities. A *Yes* in either the *Release or Exposure* column of the list activates the appropriate default model and allows the use of other available models. A *No* indicates that ChemSTEER will not assess that Source/Activity for either a release or worker exposures, as appropriate. Sources/Activities with a *No* indicator will not appear in the list of operation Sources/Activities in either the *Releases* or *Exposures* tabs, as appropriate. The indicators in these columns are ChemSTEER defaults that may be changed by clicking on the *Yes* or *No* and typing *Y* (to change to *Yes*) or *N* (to change to *No*).

### **Default Model Processing (DMP) Status**

The DMP status (i.e., the Release DMP and Exposure DMP columns) indicates whether each of the selected sources/activities have been "processed" by ChemSTEER and have had their default models selected. Be sure to read more about <u>Hierarchy of ChemSTEER Operations, Activities, and Models</u>, in particular the <u>Default Model Processing</u>.

When finished with all changes to the list of Sources/Activities to be assessed for the selected operation, click OK at the bottom of the *Update* window, and the updated list should appear in the *Sources/Activities* subtab window.

NOTE: You must select at least one Source/Activity in an operation to access ChemSTEER models.

### Set the Order of Sources/Activities Within the Operation

The default order of sources/activities is the order in which you originally added them. Ordering sources/activities will affect the display order on the Releases and Exposures tabs, and ChemSTEER will run models in the order of their associated sources/activities. The source/activity display order will not change on summary reports. ChemSTEER may offer the ability to apply a loss fraction to the amount remaining from a previous source/activity <u>in future versions</u>; however, until then, the order of sources/activities is strictly aesthetic.

To change the order of a source/activity, set focus in the Order column of the source/activity to be changed and click Move Up or Move Down. Clicking Move Up or Move Down will change the source/activity order by 1, and will automatically adjust the order numbers of the other sources/activities in the operation based on their current order.

# Operations Tab $\rightarrow$ Site Information Subtab

The Site Information subtab allows the user to record site-related (location) information for the operation. You may save the facility name, address, city, state, zip code, and county for one or more sites that are being assessed in the selected operation.

Click the *Update Site Information* button to enter site information. You can also edit and delete sites from the assessment.

<u>To add a new site</u>, click the *Add* button and enter the site's information. Click *OK* to enter the information into the assessment.

<u>To modify a site's information</u>, click on the desired site in the *Facilities* box and then click the *Modify* button. Make the desired edits and click *OK* to enter the revisions.

<u>To remove a site from the operation</u>, click on the site to be removed in the *Facilities* box and then click the *Delete* button and confirm the removal.

If the selected operation is performed at the same facility (or facilities) as the preceding operation, you may wish to copy all of the site information that was entered for the preceding operation. To do this, click the *Copy Previous Operation* button. You may then add, modify or delete the facility information as appropriate for the selected operation.

# **OPERATIONS PARAMETERS TAB**

You can use the *Operation Parameters* tab to view and/or update key mass balance and container-related parameters for each of the assessed operations. These key parameters may be used in generating default values for parameters used in models for release and exposure estimation. The Operation Parameters tab also contains the *Shared Parameters/Factors* subtab, where you can input and specify certain parameters that are shared by more than one release and/or exposure model.

The data fields in the views accessed by clicking on the subtabs in the lower half of the *Operation Parameters* tab are relevant to the Operation that is selected. The selected Operation is highlighted, and you can select another Operation by clicking on that Operation label in the list on the upper half of the *Operation* tab. To update the data fields in the subtabs (*Mass Balance, Container Parameters*, or *Shared Parameters/Factors*), click on the subtab label and then click on the *Update* button located in each subtab. An *Update* window will appear and you can click on the data field to enter the appropriate information. Clicking the *OK* button at the bottom of the window will enter the new information into the assessment.

For EACH operation, enter the *Mass Balance* subtab parameters in the *Update* window accessed using the *Update Parameters* button. Then click on the *Container Parameters* subtab. The general rules, calculations, and logic by which ChemSTEER makes mass balance-related parameter estimations are contained in the <u>Operation Parameters Tab</u>  $\rightarrow$  <u>Mass Balance Parameters Subtab</u> pages of this User Guide.

For EACH operation, view the *Container Parameter* subtab parameters for each of the subtabs as they are ordered from left to right (For *Raw Materials, For Other Materials, For Product*, and *Container Parameters by Activity*). If you wish to change any of the parameters' values, double-click on the appropriate Source/Activity name and make the change in the *Update* window accessed. For each operation, the term "Raw Material" refers to material entering the operation, whether pure chemical or chemical in a mixture, and the term "Product" refers to material leaving the operation, whether pure chemical or chemical in a mixture. The general rules, calculations, and logic by which ChemSTEER makes

container-related parameter estimations are contained in the <u>Container Parameters Guidance</u> pages of this User Guide.

When you have completed entering Container Parameters, click on the *Shared Parameters/Factors* subtab. For EACH operation, verify any necessary shared parameter values. Currently, this subtab contains the following types of shared parameters:

- Vapor Pressure Shared Parameters (e.g., Xrm, Xprod, Xother, AVPrm, AVPprod); and
- Automobile Spray Painting Shared Parameters (e.g., designation of the spray gun type, spray booth type, and mist control technology used in the operation).

Be sure to read the <u>Operation Parameters Tab  $\rightarrow$  Shared Parameters/Factors Subtab</u> topic.

# Operation Parameters Tab → Mass Balance Parameters Subtab

You can use the *Mass Balance Parameters* subtab to view and/or update key mass balance parameters for each of the assessed operations. These key mass balance parameters are used frequently in generating default values for parameters used in models for release and exposure estimation.

Since batch operations have parameters expressed 'per batch' while most release and exposure estimates are expressed per time, the *Mass Balance* subtab allows ChemSTEER to convert batch variables into time frames.

### **General Mass Balance Rules and Notes**

Rules below apply only if you perform mass balance calculations; however, you may run models without performing mass balance calculations. Default settings are described in the <u>Mass Balance Basis</u> <u>Selection</u>.

ChemSTEER currently rounds values that are required to be an integer to the nearest integer value (with the exception that values less than one are always be rounded to one). In future versions, ChemSTEER may include recommendations for mitigating rounding errors.

Some user inputs can result in discrepancies in the mass balance logic. Some discrepancies will result in warnings and/or warning flags; however, ChemSTEER generally allows you to proceed despite apparent imbalances identified in the mass balance logic.

Some user inputs can result in broad effects on other operations. For example, Yprod is a default value for subsequent operations. If Yprod for a given operation (e.g., paint formulation) is changed after a subsequent operation (e.g., paint application) is assessed, the overall mass balance and assessed exposures and releases of the subsequent operation may contain discrepancies that would require your correction. ChemSTEER will warn you that changing Yprod can impact appropriateness of parameters' values in the mass balances and their applications in models in subsequent operations.

If you skip the Mass Balance Parameters tab and proceed directly to an activity/model, ChemSTEER will assume batch operations as the default. These assumptions will impact the parameters and associated units displayed on the model input parameters screens. Note: ChemSTEER also shows several "placeholder calculate buttons" for several of the mass balance input parameters. These buttons are currently disabled for all of these input parameters, except for DMIchem and DMOchem.

### **Key Mass Accounting Parameters**

DMIchem:	Daily Mass Input of Chemical (kg/site-day)
DMOchem:	Daily Mass Output of Chemical (kg/site-day)
BMIchem:	Batch Mass Input of Chemical (kg/site-batch)
BMOchem:	Batch Mass Output of Chemical (kg/site-batch)
DMIrm:	Daily Mass Input of Raw Material containing the Chemical (kg/site-day)
DMOprod:	Daily Mass Output of Product containing the Chemical (kg/site-day)
BMIrm:	Batch Mass Input of Raw Material containing the Chemical (kg/site-batch)
BMOprod:	Batch Mass Output of Product containing the Chemical (kg/site-batch)
Yrm:	Weight Fraction of Chemical in Raw Material (0 < Yrm < 1)
Yprod:	Weight Fraction of Chemical in Product (0 < Yprod < 1)
NS:	Number of sites (integer > 0)
OD:	Operating days per site per year (days/site-yr) (integer > 0 and < 365, OD < ODmax)
Nby :	Number of batches per site per year (batches/site-year) (integer > 0)

### **Additional Continuous Operation Parameters**

HMIchem:	Hourly mass input of chemical (kg/site-hr)
HMOchem:	Hourly mass output of chemical (kg/site-hr)
HD:	Hours per day (0 < HD < 24; default = 24 hours)

### Additional Batch-Related Parameters

HB:	Hours per batch (hours/batch) (default HB = 24, 0 < HB < 8760)
ODmax:	Maximum number of operating days possible for the batch operation (days/year) (default ODmax = 365, integer > 0 and < 365)
Nbld:	Number of batches per line per day (batches/line-day) (Nbld < 24/HB and 0 < Nbld < Nby)
Ls:	Number of processing lines per site (lines/site) (default Ls = 1, integer > 0)
Nbd:	Number of batches per site-day (batches/site-day)

These parameters are used to perform mass balance calculations on the three ChemSTEER Mass Balance Parameters subtabs as described in the sections below:

- Mass Balance Basis Selection
- <u>Specify Mass Balance Input Parameters</u>
- <u>Specify Other Batch Parameters</u> (hidden if *Continuous* operation is chosen by the user)

NOTE: Be aware that changing certain parameters on the Mass Balance Parameters Subtab will affect the container-related calculations and release and exposure model estimates. Be sure to read about <u>Hierarchy of ChemSTEER Operations</u>, <u>Activities</u>, <u>and Models</u>.

# Mass Balance Basis Selection

You will make the following two selections (type of operation and material basis) before entering values in subsequent mass balance screens:

Choice 1: Select type of Operation

- [ ] Continuous Operation
- [] Batch Operation

The default setting for Choice 1 is *Batch Operation* for any user-defined operation and for industry-specific operations, unless otherwise specified.

Choice 2: Use the operation's raw material or product as the basis for mass balance

- [ ] Raw Material (raw materials entering the operation)
- [ ] Product (product leaving the operation)

The default settings for Choice 2 are as follows:

- Product for User-Defined Manufacturing (Product is not available for User-Defined Use); and
- Raw Material for User-Defined Processing and User-Defined Use, as well as for industryspecific operations, unless otherwise specified (Raw Material is not available for User-Defined Manufacturing).

The default settings described for Choice 1 and Choice 2 are used when you skip the Mass Balance Parameters tab and proceed directly to a source or activity and its model(s). These assumptions will impact the parameters and associated units displayed on the model input parameters screens.

### Specify Mass Balance Input Parameters

The following four combinations describe the possible user decisions and subsequent calculations made by ChemSTEER based on the selections made on the <u>Mass Balance Basis Selection</u>.

Click on one of the following bases (selected in the <u>Mass Balance Basis Selection</u> subtab) to read more about the default settings and calculations:

Type of Operation: Continuous; Basis: Raw Material

Type of Operation: Continuous; Basis: Product

Type of Operation: Batch; Basis: Raw Material

Type of Operation: Batch; Basis: Product

### Type of Operation: Continuous; Basis: Raw Material

NOTE: User-defined Manufacturing cannot use Raw Material as a basis.

This screen has four parameter groupings as follows:

### First Parameter Grouping (you must specify at least one parameter):

NS:	Number of sites
OD:	Total number of operating days per year at each site

### Second Parameter Grouping (you must specify at least one parameter):

Yrm:	Weight fraction of chemical in raw material
DMIrm:	Daily mass input of raw material containing the chemical (kg/site-day)

### Third Parameter Grouping:

DMIchem:	Dail	v mass in	put of	chemical (	kø	/site-dav)
Divitchent.	Dan	y 111033 111	putor	chemicar	<u>15</u> /	Site day

For user-defined operations, it is <u>recommended</u> that you specify exactly three parameters from the first three groupings (including at least one parameter from the first grouping and at least one parameter from the second grouping). You *specify* parameters by clicking the fix box to the left of the parameter and entering a positive non-zero value. For industry-specific operations, some of these mass balance parameters will have default values.

You may elect to enter less than three parameters in the *Specify Mass Balance Input Parameters* subtab and ChemSTEER will allow you to move on to subsequent screens.

NOTE: Since many of the mass balance parameters are used as default values and used in several of the calculations performed in ChemSTEER, not entering/calculating all of the mass balance parameters may prevent some calculations from being performed in the assessment.

A primary calculation in the Mass Balance Parameter subtabs is DMIchem (daily mass input of chemical). The following rules describe the ChemSTEER default calculations of DMIchem, based on your specifications:

If you specify NS and OD, and either Yrm or DMIrm:

DMIchem = PVop / NS / OD

where PVop = the production volume associated with the operation.

If you specify Yrm and DMIrm, and either NS or OD:

### DMIchem = Yrm \* DMIrm

You may utilize an hourly input rate for the chemical (HMIchem) and operation hours per day (HD) to calculate DMIchem.

To execute this calculation, first click the fix box to the left of DMIchem, then click the *Calculate* button to the right. Clicking the *Calculate* button launches the *Calculate DMIchem* update window, wherein you enter values for the following input parameters:

HMIchem:	Hourly mass input of chemical (kg/site-hr)
HD:	Hours per day (0 < HD < 24; default = 24 hours)

After entering these two values, click the *Calculate* button in the update window to execute the following equation to calculate DMIchem:

DMIchem = HMIchem (kg/site-hr) x HD (hours/day)

Clicking *OK* will cause the newly calculated value of DMIchem to overwrite any existing value that was displayed on the *Specify Mass Balance Input Parameters* subtab.

If you directly specify DMIchem, DMIchem will be set equal to the value you provide.

Any values entered for HMIchem and HD will be retained on the *Calculate DMIchem* update window.

**NOTE:** For operations THAT HAVE A PRECEDING OPERATION, the default values for Yrm (current operation) = Yprod FROM THE PRECEDING OPERATION.

If a mass accounting discrepancy is calculated by ChemSTEER based on the following equations, you will be warned with a pop-up message but allowed to continue. In addition, a warning note will appear at the bottom of the *Specify Mass Balance Input Parameters* subtab.

<u>Parameter</u>	Percent Error Value Calculation
NS	%error = (NSrounded / NScalc - 1) * 100
OD	%error = (ODrounded / ODcalc - 1) * 100

### Fourth Parameter Grouping:

Yprod:	Weight fraction of chemical in product
DMOprod:	Daily mass output of product containing the chemical (kg/site-day)
DMOchem:	Daily mass output of chemical (kg/site-day)

For *processing* operations, the default values for the fourth grouping are as follows:

Yprod (current operation) = Yrm (current operation)

DMOprod (current operation) = DMIrm (current operation)

DMOchem (current operation) = DMIchem (current operation)

For *use* operations, the default values for the fourth grouping are as follows:

Yprod (current operation) = 0 DMOprod (current operation) = 0 DMOchem (current operation) = 0

**NOTE:** No defaults are available for *manufacturing* operations since User-defined Manufacturing cannot use Raw Material as a basis.

You may then change up to two of the parameters in the fourth grouping. For industry-specific operations, some of these mass balance parameters will have default values.

After making these changes, ChemSTEER will recalculate the value of the parameter for which you click the *Recalc* button using the following relationship:

DMOprod = DMOchem / Yprod.

The *Recalc* button is located to the right of the text box for each parameter in the fourth grouping. If you change one or more parameters in the fourth grouping, you will not be allowed to exit the screen without clicking the *Recalc* button for at least one parameter or clicking *Cancel* to discard ALL changes (including those made to parameters in the first three groupings).

If you change values in the fourth grouping, the values in the first three groupings are not affected (i.e., if DMOchem ...DMIchem in a processing operation, ChemSTEER will not make changes to resolve the apparent discrepancy). ChemSTEER will warn you if this apparent discrepancy occurs.

### Type of Operation: Continuous; Basis: Product

NOTE: User-defined Use cannot use Product as a basis.

This screen has four parameter groupings as follows:

### First Parameter Grouping (you must specify at least one parameter):

NS:	Number of sites
OD:	Total number of operating days per year at each site

### Second Parameter Grouping (you must specify at least one parameter):

Yprod:	Weight fraction of chemical in product
DMOprod:	Daily mass output of product containing the chemical (kg/site-day)

### Third Parameter Grouping:

DMOchem: Daily mass output of chemical (kg/site-day)

For user-defined operations, it is <u>recommended</u> that you specify exactly three parameters from the first three groupings (including at least one parameter from the first grouping and at least one parameter from the second grouping). You *specify* parameters by clicking the fix box to the left of the parameter and entering a positive non-zero value. For industry-specific operations, some of these mass balance parameters will have default values.

You may elect to enter less than three parameters in the *Specify Mass Balance Input Parameters* subtab and ChemSTEER will allow you to move on to subsequent screens.

NOTE: Since many of the mass balance parameters are used as default values and used in several of the calculations performed in ChemSTEER, not entering/calculating all of the mass balance parameters may prevent some calculations from being performed in the assessment.

A primary calculation in the Mass Balance Parameter subtabs is DMOchem (daily mass output of chemical). The following rules describe the ChemSTEER default calculations of DMOchem, based on user specifications:

If you specify NS and OD, and either Yprod or DMOprod:

DMOchem = PVop / NS / OD

where PVop = the production volume associated with the operation.

If you specify Yprod and DMOprod, and either NS or OD:

DMOchem = Yprod \* DMOprod

You may utilize an hourly output rate for the chemical (HMOchem) and operation hours per day (HD) to calculate DMOchem.

To execute this calculation, first click the fix box to the left of DMOchem, then click the *Calculate* button to the right. Clicking the *Calculate* button launches the *Calculate DMOchem* update window, wherein you enter values for the following input parameters:

HMOchem:	Hourly mass output of chemical (kg/site-hr)
HD:	Hours per day (0 < HD < 24; default = 24 hours)

After entering these two values, click the *Calculate* button in the update window to execute the following equation to calculate DMOchem:

DMOchem = HMOchem (kg/site-hr) x HD (hours/day)

Clicking *OK* will cause the newly calculated value of DMOchem to overwrite any existing value that was displayed on the *Specify Mass Balance Input Parameters* subtab.

If you directly specify DMOchem, DMOchem will be set equal to the value you provided.

Any values entered for HMOchem and HD will be retained on the *Calculate DMOchem* update window.

If a mass accounting discrepancy is calculated by ChemSTEER based on the following equations, you will be warned with a pop-up message but allowed to continue. In addition, a warning note will appear at the bottom of the *Specify Mass Balance Input Parameters* subtab.

<u>Parameter</u>	Percent Error Value Calculation
NS	%error = (NSrounded / NScalc - 1) * 100
OD	%error = (ODrounded / ODcalc - 1) * 100

### Fourth Parameter Grouping:

Yrm:	Weight fraction of chemical in raw material
DMIrm:	Daily mass output of raw material containing the chemical (kg/site-day)
DMIchem:	Daily mass input of chemical (kg/site-day)

For *processing* operations, THAT HAVE NO PRECEDING OPERATION, the default values for the fourth grouping are as follows:

Yrm (current operation) = Yprod (current operation)

DMIrm (current operation) = DMOprod (current operation)

DMIchem (current operation) = DMOchem (current operation)

For *processing* operations, THAT HAVE A PRECEDING OPERATION, the default values for the fourth grouping are as follows:

Yrm (current operation) = Yprod FROM THE PRECEDING OPERATION

DMIchem (current operation) = DMOchem (current operation)

For *manufacturing* operations, the default values for the fourth grouping are as follows:

Yprod (current operation) = 0

DMOprod (current operation) = 0

DMOchem (current operation) = 0

**NOTE:** No defaults are available for *use* operations since User-defined Use cannot use Product as a basis.

You may then change up to two of the parameters in the fourth grouping. For industry-specific operations, some of these mass balance parameters will have default values.

After making these changes, ChemSTEER will recalculate the value of the parameter for which you click the *Recalc* button using the following relationship:

DMrm = DMIchem / Yrm.

The *Recalc* button is located to the right of the text box for each parameter in the fourth grouping. If you change one or more parameters in the fourth grouping, you will not be allowed to exit the screen without clicking the *Recalc* button for at least one parameter or clicking *Cancel* to discard ALL changes (including those made to parameters in the first three groupings).

If you change values in the fourth grouping, the values in the first three groupings are not affected (i.e., if DMIchem ...DMOchem in a processing operation, ChemSTEER will not make changes to resolve the apparent discrepancy). ChemSTEER will warn you if this apparent discrepancy occurs.

# Type of Operation: Batch; Basis: Raw Material

NOTE: User-defined Manufacturing cannot use Raw Material as a basis.

This screen has four parameter groupings as follows:

### First Parameter Grouping (you must specify at least one parameter):

NS:	Number of sites
Nby:	Total number of batches per year at each site

### Second Parameter Grouping (you must specify at least one parameter):

Yrm:	Weight fraction of chemical in raw material
BMIrm:	Batch mass input of raw material containing the chemical (kg/batch)

### Third Parameter Grouping:

BMIchem: Batch mass input of chemical (kg/batch)

For user-defined operations, it is <u>recommended</u> that you specify exactly three parameters from the first three groupings (including at least one parameter from the first grouping and at least one parameter from the second grouping). You *specify* parameters by clicking the fix box to the left of the parameter and entering a positive non-zero value. For industry-specific operations, some of these mass balance parameters will have default values.

You may elect to enter less than three parameters in the Specify Mass Balance Input Parameters subtab and ChemSTEER will allow you to move on to subsequent screens.

**NOTE**: Since many of the mass balance parameters are used as default values and used in several of the calculations performed in ChemSTEER, not entering/calculating all of the mass balance parameters may prevent some calculations from being performed in the assessment.

A primary calculation in the Mass Balance Parameter subtabs is BMIchem (batch mass input of chemical). The following rules describe the ChemSTEER default calculations of BMIchem, based on user specifications:

If you specify NS and Nby, and either Yrm or BMIrm:

BMIchem = PVop / NS / Nby

where PVop = the production volume associated with the operation.

If you specify Yrm and BMIrm, and either NS or Nby:

BMIchem = Yrm \* BMIrm

If you specify BMIchem, BMIchem will be set equal to the value you provide.

**NOTE:** For operations THAT HAVE A PRECEDING OPERATION, the default values for Yrm (current operation) = Yprod FROM THE PRECEDING OPERATION.

If a mass accounting discrepancy is calculated by ChemSTEER based on the following equations, you will be warned with a pop-up message but allowed to continue. In addition, a warning note will appear at the bottom of the *Specify Mass Balance Input Parameters* subtab.

<u>Parameter</u>	Percent Error Value Calculation
NS	%error = (NSrounded / NScalc - 1) * 100
Nby	%error = (Nbyrounded / Nbycalc - 1) * 100

### Fourth Parameter Grouping:

Yprod:	Weight fraction of chemical in product
BMOprod:	Batch mass output of product containing the chemical (kg/site-day)
BMOchem:	Batch mass output of chemical (kg/site-day)

For *processing* operations, the default values for the fourth grouping are as follows:

Yprod (current operation) = Yrm (current operation)BMOprod (current operation) = BMIrm (current operation)BMOchem (current operation) = BMIchem (current operation)

For *use* operations, the default values for the fourth grouping are as follows:

Yprod (current operation) = 0 BMOprod (current operation) = 0 BMOchem (current operation) = 0

**NOTE:** No defaults are available for *manufacturing* operations since User-defined Manufacturing cannot use Raw Material as a basis.

You may then change up to two of the parameters in the fourth grouping. For industry-specific operations, some of these mass balance parameters will have default values.

After making these changes, ChemSTEER will recalculate the value of the parameter for which you click the *Recalc* button using the following relationship:

BMOprod = BMOchem / Yprod.

The *Recalc* button is located to the right of the text box for each parameter in the fourth grouping. If you change one or more parameters in the fourth grouping, you will not be allowed to exit the screen without clicking the *Recalc* button for at least one parameter or clicking *Cancel* to discard ALL changes (including those made to parameters in the first three groupings).

If you change values in the fourth grouping, the values in the first three groupings are not affected (i.e., if BMOchem ...

BMIchem in a processing operation, ChemSTEER will not make changes to resolve the apparent discrepancy). ChemSTEER will warn you if this apparent discrepancy occurs.

Continue to Specify Other Batch Parameters subtab

### Type of Operation: Batch; Basis: Product

NOTE: User-defined Use cannot use Product as a basis.

This screen has four parameter groupings as follows:

### First Parameter Grouping (you must specify at least one parameter):

NS:	Number of sites
Nby:	Total number of batches per year at each site

### Second Parameter Grouping (you must specify at least one parameter):

Yprod:	Weight fraction of chemical in product
BMOprod:	Batch mass output of product containing the chemical (kg/batch)

#### **Third Parameter Grouping:**

BMOchem: Batch mass output of chemical (kg/batch)

For user-defined operations, it is <u>recommended</u> that you specify exactly three parameters from the first three groupings (including at least one parameter from the first grouping and at least one parameter from the second grouping). You *specify* parameters by clicking the fix box to the left of the parameter and entering a positive non-zero value. For industry-specific operations, some of these mass balance parameters will have default values.

You may elect to enter less than three parameters in the Specify Mass Balance Input Parameters subtab and ChemSTEER will allow you to move on to subsequent screens.

**NOTE**: Since many of the mass balance parameters are used as default values and used in several of the calculations performed in ChemSTEER, not entering/calculating all of the mass balance parameters may prevent some calculations from being performed in the assessment.

A primary calculation in the Mass Balance Parameter subtabs is BMOchem (batch mass output of chemical). The following rules describe the ChemSTEER default calculations of BMIchem, based on your specifications:

If you specify NS and Nby, and either Yprod or BMOprod:

BMOchem = PVop / NS / Nby

where PVop = the production volume associated with the operation.

If you specify Yprod and BMOprod, and either NS or Nby:

BMOchem = Yprod \* BMOprod

If you specify BMOchem, BMOchem will be set equal to the value you provide.

If a mass accounting discrepancy is calculated by ChemSTEER based on the following equations, you will be warned with a pop-up message but allowed to continue. In addition, a warning note will appear at the bottom of the *Specify Mass Balance Input Parameters* subtab.

<u>Parameter</u>	Percent Error Value Calculation
NS	%error = (NSrounded / NScalc - 1) * 100
Nby	%error = (Nbyrounded / Nbycalc - 1) * 100

### Fourth Parameter Grouping:

Yrm:	Weight fraction of chemical in raw material
BMIrm:	Batch mass input of raw material containing the chemical (kg/site-day)
BMIchem:	Batch mass input of chemical (kg/site-day)

For *processing* operations THAT HAVE NO PRECEDING OPERATION, the default values for the fourth grouping are as follows:
Yrm (current operation) = Yprod (current operation)

BMIrm (current operation) = BMOprod (current operation)

BMIchem (current operation) = BMOchem (current operation)

For *processing* operations THAT HAVE A PRECEDING OPERATION, the default values for the fourth grouping are as follows:

Yrm (current operation) = Yprod FROM THE PRECEDING OPERATION

BMIchem (current operation) = BMOchem (current operation)

For *manufacturing* operations, the default values for the fourth grouping are as follows:

Yrm (current operation) = 0 BMIrm (current operation) = 0 BMIchem (current operation) = 0

**NOTE:** No defaults are available for *use* operations since User-defined Use cannot use Product as a basis.

You may then change up to two of the parameters in the fourth grouping. For industry-specific operations, some of these mass balance parameters will have default values.

After making these changes, ChemSTEER will recalculate the value of the parameter for which you click the *Recalc* button using the following relationship:

BMrm = BMIchem / Yrm.

The *Recalc* button is located to the right of the text box for each parameter in the fourth grouping. If you change one or more parameters in the fourth grouping, you will not be allowed to exit the screen without clicking the *Recalc* button for at least one parameter or clicking *Cancel* to discard ALL changes (including those made to parameters in the first three groupings).

If you change values in the fourth grouping, the values in the first three groupings are not affected (i.e., if BMIchem ...

BMOchem in a processing operation, ChemSTEER will not make changes to resolve the apparent discrepancy). ChemSTEER will warn you if this apparent discrepancy occurs.

Continue to Specify Other Batch Parameters subtab

# Specify Other Batch Parameters

This screen is used for *Batch* operations only. You cannot access this tab until a value for at least the Nby parameter (number of batches per site, per year) has been entered or calculated in the <u>Specify</u>

<u>Mass Balance Input Parameters</u> subtab for *Batch* operations. This screen has three parameter groupings as follows:

#### First Parameter Grouping:

Nby:	Number of batches/site-year (carried forward from Specify Mass Input Balance Parameters subtab, read-only – cannot be specified or changed
	on this screen).
HB:	Hours per batch
ODmax:	Maximum possible operating days

Nby is the same value specified or calculated from the Specify Mass Balance Input Parameters subtab.

You should specify HB and change ODmax, if appropriate.

#### Second Parameter Grouping: (parameters calculated based on the logic below)

Nbld:	Number of batches per line per day
Ls:	Processing lines per site
OD:	Operating days per year

The second parameter groupings are calculated based on defaults or recalculated if you change a first parameter grouping and click off of the parameter.

# Third Parameter Grouping

Nbd: Number of batches/site-day (read-only - cannot be specified or changed) = Nbld \* Ls

You *specify* parameters by entering a positive non-zero value and clicking the checkbox for the parameter. Based upon your specifications from the first parameter grouping, ChemSTEER calculates default values for the second and third parameter groupings as follows:

If HB # 24 AND Nby <= ODmax, then ChemSTEER defaults to the following:

Ls = 1 Nbld = 1 OD = Nby

If **HB >24 and/or Nby >365 AND (HB\*Nby)/24 <= ODmax**, then ChemSTEER defaults are the following:

```
Ls =1
OD = (HB*Nby / Ls) / 24
Nbld = Nby / OD / Ls
```

If **HB >24 and/or Nby >365 and/or (HB\*Nby)/24 > ODmax**, then ChemSTEER defaults to the following:

Increase Ls by one until (HB\*Nby / Ls) / 24 is less than or equal to ODmax OD = (HB\*Nby / Ls) / 24 Nbld = Nby / OD / Ls

You may then change up to two of the parameters in the second parameter grouping. After making these changes, ChemSTEER will recalculate the value of the parameter for which you click the *Re-Calculate* button using the following relationship:

OD = Nby / Nbld / Ls.

If a mass accounting discrepancy is calculated by ChemSTEER based on the parameters the following equations, you will be warned with a pop-up message but allowed to continue. In addition, a warning note will appear at the bottom of this mass balance screen.

<u>Parameter</u>	Percent Error Value Calculation	
Ls	% error = (Lsrounded / Lscalc - 1) * 100	
OD	% error = (ODrounded / ODcalc - 1) * 100	

The *Re-Calculate* button is next to the text box for each parameter in the second grouping. If you change one or more parameters in the second grouping, you will not be allowed to exit the screen without pressing the *Re-Calculate* button for at least one parameter or pressing the *Cancel* button to discard ALL changes (including those made to parameters in the first grouping).

# Operation Parameters Tab → Container Parameters Subtab

You can use the *Container Parameter* subtab to view and/or update key container-related parameters for each of the assessed operations. These key container parameters are used frequently in generating default values for parameters used in models for release and exposure estimation.

For EACH operation, view the *Container Parameter* subtab parameters for each of the subtabs as they are ordered from left to right (*For Raw Materials, For Other Materials, For Product,* and *Container Parameters by Activity*). If you wish to change any of the parameters' values, double-click on the appropriate Source/Activity name and make the change in the *Update* window accessed.

The general rules, calculations, and logic by which ChemSTEER makes container parameterrelated estimations are contained in the <u>Container Parameters Guidance</u> page of this User Guide.

# **Container Parameters Guidance**

The logic and parameters are described below for the ChemSTEER Container Parameters subtab when the user clicks the *Update Parameters* button.

This tab is used to verify and/or specify container-related parameters that are sometimes relevant to both release models and exposure models.

#### **General Container Parameter Rules and Notes**

Rules below apply only if user performs container parameter calculations; however, the user may run models without performing container parameter calculations. ChemSTEER will generate some default values without any user action under the Container Parameter subtabs.

ChemSTEER currently rounds values that are required to be an integer to the nearest integer value (with the exception that values less than one are always be rounded to one). In future versions, ChemSTEER may include "recommendations" for mitigating rounding errors.

Some user inputs can result in discrepancies in the mass balance and/or container logic. Some discrepancies will result in warnings and/or warning flags. However, ChemSTEER generally allows the user to proceed despite apparent imbalances identified in the mass balance logic.

Some user inputs can result in broad effects on other operations. For example, Yprod is a default value for subsequent operations. If Yprod for a given operation (e.g., paint formulation) is changed after a subsequent operation (e.g., paint application) is assessed, the overall mass balance, container parameters, and assessed exposures and releases of the subsequent operation may contain discrepancies that would require user correction. ChemSTEER will warn the user that changing Yprod can impact appropriateness of parameters' values in the mass balances and their applications in container logic and models in subsequent operations.

# **Key Container Parameters**

- fc: Fraction of total volume (raw material or product) shipped in this container, dimensionless (0 < fc < 1)
- Vc: Container volume (gal)
- i: Activity designator (can be used for any activities using raw material (rm), product (prod), or other user-defined material)
- Di: Density of material handled in activity i (kg/L) (default Di = 1, except Drm (current operation) = Dprod from the preceding operation)
- Yi: Weight fraction of chemical in material handled in activity i, dimensionless (0 < Yi < 1)
- MCi: Mass of material in container handled in activity i (kg/container)
- OD: Days per site per year for the operation (days/year) (read-only from Mass Balance)
- Ncy: Number of containers per site per year (containers/site-year)
- ODa: Days per site per year for the activity (days/yr) (integer > 0 and < 365)
- Ncd: Number of containers per site per day (containers/site-day) (Ncd < Ncy)
- r: Rate of unloading/loading containers (containers/hour)
- OHa: Hours per day for the activity (hours/day) (0 < OHa < 24)

These parameters are used to perform container-handling calculations on the ChemSTEER Container Parameters subtabs, as described in the links below:

• Verify/Select Container Parameters

# • <u>Verify/Select Container Parameter by Activity</u>

NOTE: Be aware that changing certain parameters on the Container Parameters subtab will affect the release and exposure model estimates. Be sure to read about <u>Hierarchy of ChemSTEER</u> <u>Operations, Activities, and Models</u>.

# Verify/Select Container Parameters

The following three subtabs are displayed on the Container Parameters subtab:

- For Raw Material
- For Product, and
- For Other Material.

Tables in these three tabs are populated based on container-related activities and other activities that are potentially container-related (e.g., miscellaneous sources and activities) selected for the operation. ChemSTEER places the activity in the "most logical" tab for the purpose of determining initial sets of default values and calculations. This placement is shown in the table below. The appearance of an activity being in an inappropriate category simply means that you may have to override the default values to send more appropriate parameter values to models that use those parameters.

Activity Name	Default Subtab for Container Parameters		
Category Name: Cleaning Liquid Residuals from Transport Containers/Vessels			
Cleaning Liquid Residuals from Bottles Used to Transport the Raw Material	Raw Material		
Cleaning Liquid Residuals from Small Containers Used to Transport the Raw Material	Raw Material		
Cleaning Liquid Residuals from Drums Used to Transport the Raw Material	Raw Material		
Cleaning Liquid Residuals from Totes Used to Transport the Raw Material	Raw Material		
Cleaning Liquid Residuals from Tank Trucks Used to Transport the Raw Material	Raw Material		
Cleaning Liquid Residuals from Rail Cars Used to Transport the Raw Material	Raw Material		
Cleaning Liquid Residuals from Containers Used to Transport the Raw Material	Raw Material		
Cleaning Liquid Residuals from Bottles Used to Transport the Raw Material	Product		
Cleaning Liquid Residuals from Small Containers Used to Transport the Raw Material	Product		
Cleaning Liquid Residuals from Drums Used to Transport the Raw Material	Product		
Cleaning Liquid Residuals from Totes Used to Transport the Raw Material	Product		
Cleaning Liquid Residuals from Tank Trucks Used to Transport the Raw Material	Product		
Cleaning Liquid Residuals from Rail Cars Used to Transport the Raw Material	Product		
Cleaning Liquid Residuals from Containers Used to Transport the Raw Material	Product		
Cleaning Liquid Residuals from Storage/Transport Vessels (User-Defined)	Other Material		
Category Name: Cleaning Solid Residuals from Transport Containers/Vessels			
Cleaning Solid/Powder Residuals from Containers Used to Transport the Raw Material	Raw Material		
Cleaning Solid/Powder Residuals from Containers Used to Transport the Product	Product		
Cleaning Solid Residuals from Storage/Transport Vessels (User-Defined)	Other Material		
Category Name: Loading Liquids into Transport Containers/Vessels			
Loading Liquid Product into Bottles	Product		
Loading Liquid Product into Small Containers	Product		
Loading Liquid Product into Drums	Product		
Loading Liquid Product into Totes	Product		
Loading Liquid Product into Tank Trucks	Product		
Loading Liquid Product into Rail Cars	Product		
Loading Liquid Product into Containers	Product		
Loading Liquid Raw Materials into Containers	Raw Material		
Loading Liquid into Storage/Transport Vessels (User-Defined)	Other Material		
Category Name: Loading Solids into Transport Containers/Vessels			
Loading Solid Product into Transport Containers	Product		
Loading Solid Raw Material into Transport Containers	Raw Material		
Loading Solids into Storage/Transport Vessels (User-Defined)	Other Material		
Category Name: Unloading Liquids into Transport Containers/Vessels			
Unloading Liquid Raw Material from Bottles	Raw Material		
Unloading Liquid Raw Material from Small Containers	Raw Material		
Unloading Liquid Raw Material from Drums	Raw Material		

# **ChemSTEER Placement of Sources and Activities into Container Groupings**

Unloading Liquid Raw Material from Totes	Raw Material		
Unloading Liquid Raw Material from Tank Trucks	Raw Material		
Unloading Liquid Raw Material from Rail Cars	Raw Material		
Unloading Liquid Raw Material from Containers	Raw Material		
Unloading Liquid Product from Containers	Product		
Unloading Liquid from Storage/Transport Containers (User-Defined)	Other Material		
Category Name: Unloading Solids into Transport Containers/Vessels			
Unloading Solid Raw Materials from Transport Containers	Raw Material		
Unloading Solid Product from Transport Containers	Product		
Unloading Solids from Storage/Transport Containers (User-Defined)	Other Material		

These three tabs allow you to view and change several operation-related parameters for each activity, including:

- Fractions of annual operation volume relevant to the activity,
- Volumes of storage and transport containers,
- Densities for the material(s),
- Mass of material in a container, and
- Weight fraction(s) of the chemical in the material(s).

Activities involving liquids are assigned default values by ChemSTEER. You may update values of parameters on the For Raw Material, For Product, and For Other Material subtabs.

Total fractions of annual operation volumes for each of the raw material and product should normally sum to 1. If you exceed the sum of 1 for raw materials or product, you will be warned with a pop-up message but allowed to continue.

ChemSTEER uses initial default value of *fc* based on the following equation:

fc = 1/(number of activities for either raw material, product, or other material, as appropriate)

For all activities, the defaults for Yi are summarized below: Yi = Yrm for activities handling raw material or other material. Yi = Yprod for activities handling product.

# Liquid-Handling Activity Defaults

For activities involving *liquids*, default values for *Vc* and Unloading/Loading Rates (r) are summarized in the table below:

Vessel Name	Default Volume (Vc), [gal]	Range of Volumes [gal]	Container Unload/Load Rate (r), [containers/hr]	Average Unload/Load Rate, [gal/min]
Bottles	1	<5		
Conservative Case Typical Case			90 60	1.5 1.0
Small Containers	5	≥ 5 to < 20		
Conservative Case			90	7.5
Typical Case			60	5.1
Drums	55	≥ 20 to < 100		
Conservative Case			30	27.5
Typical Case			20	18.3
Totes	550	≥ 100 to < 1,000		
Conservative Case			30	27.5
Typical Case			20	18.3
Tank Truck	5,000	≥ 1,000 to < 10,000		
Conservative Case			2	167
Typical Case			2	167
Rail Car	20,000	≥ 10,000		
Conservative Case			1	333
Typical Case			1	333

Table 1. Default Values for Container Volumes (Vc) and Unloading/Loading Rates (r) for Activities
Involving Liquids

Source: portions from USEPA, 1991, Table 4-11.

The defaults for *Di* are summarized below:

Di = Drm for activities handling raw material or other material

Di = Dprod for activities handling product.

The overall ChemSTEER default value for *Di* is one kilogram per liter (1 kg/L), except Drm (current operation) = Dprod from the *preceding* operation.

ChemSTEER calculates *MCi* based on the values of *Vc* and *Di* using the following equation:

MCi = Vc \* Di \* 3.785 L/gal

You may delete the values of *Vc* and *Di* to enter a new value for *MCi* directly. Alternatively, you may change either *Vc* or *Di* and ChemSTEER will update the value of *MCi* based on the equation above.

# Solid-Handling Activity Defaults:

For activities involving *solids*, there are no default values for *Vc*, *Di* and *MCi*. You must either specify a value for *MCi* (Vc and Di left blank) or specify values for *Vc* and *Di*. ChemSTEER will then calculate *MCi* using the following equation:

# Verify/Select Container Parameter by Activity

This tab allows you to view or change the activity-specific parameters listed in the table below. The default values for each of the parameters are presented in <u>Table 1 above</u>.

Activity-Specific Parameter	Definition	Default Value
Ncy	Number of containers per site per year	(PVop*fc)/(NS*Yi*MCi)
ODa	Days per site per year for the activity	Nby (only if batch operation and Nbd <1), otherwise OD
Ncd	Number of containers per site per day	Ncy/ODa
R	Rate of unloading/loading containers (containers/hour)	Typical case value from Table 2, based on container size
ОНа	Hours per day for the activity	Ncd.r

# Activity-Specific Parameters and Default Values

This subtab displays three parameter groupings, as follows:

# First Parameter Grouping (you may select up to two parameters):

Ncy (number of containers per site-year)

ODa (days per site-year for the container-related activity)

Second Parameter Grouping (you may select up to two parameters total in the Second and Third Groupings):

Ncd (number of containers per site-day)

Third Parameter Grouping (you may select up to two parameters total in the Second and Third Groupings):

r (load/unload rate, containers per hour) OHa (hours per site-day for the container-related activity)

You may revise the default values calculated by ChemSTEER. To make revisions, you must select a total of exactly three parameters that ChemSTEER should use to calculate the remaining two parameters. You select parameters using one of the following options:

- To retain the default value, click the checkbox for the parameter; or
- To change the default value, enter a positive non-zero value and then click the checkbox for the parameter.

Based on the selected parameters' values, ChemSTEER will recalculate the values of the remaining parameters using the following equations:

Ncd = Ncy/ODa OHa = Ncd/r If a mass accounting discrepancy is calculated by ChemSTEER based on the following equations, you will be warned with a pop-up message but allowed to continue. The warning note at the bottom of the screen will appear on this container parameters screen.

<u>Parameter</u>	Error Cause	Percent Error Value Calculation
ODa	rounding	%error = (ODarounded/ODacalc - 1) * 100
Ncy	user-selected values	%error = [Ncy/((PVop * fc)/(NS * Yi * MCi)) - 1] * 100

# Operation Parameters Tab → Shared Parameters/Factors Subtab

The logic and parameters are described below for the ChemSTEER *Operation Parameters* tab, *Shared Parameters/Factors* subtab when the user clicks the *Update Parameters* button.

This tab is used to verify and/or specify parameters and factors that are shared by more than one release and/or exposure model used within an operation. These are additional parameters that are not specified in the *Chemical* tab, *Operations* subtabs, or the other *Operation Parameters* subtabs (i.e., Mass Balance and Container Parameters).

NOTE: Be aware that changing certain parameters on this subtab will affect the release and exposure model estimates. Be sure to read about <u>Hierarchy of ChemSTEER Operations, Activities, and</u> <u>Models</u>.

# **General Shared Parameters/Factors Rules and Notes**

The rules below apply only if the user performs calculations and/or enters values under this subtab; however, the user may run models without entering/performing calculations under this subtab. Default values will be generated by ChemSTEER without any user action.

Shared parameters or factors for models specific to a particular industry operation (e.g., spray gun type for the *Automotive OEM* and *Refinishing Spray Coating* operations) will only appear as preselected by default when the particular operation is selected on the list of assessed operations. Such parameters are included in the discussion of the logic for the appropriate industry-specific operation (in the User Guide's *ChemSTEER Methods and Models, Industry-Specific Operations* topics).

The adjusted vapor pressure range values (AVPlow and AVPhigh) used for activating the vapor models for the assessment appear in this subtab. Shared parameters for vapor-related models (e.g., vapor generation release models and the mass balance inhalation model) will be preselected by default, based on preselection default conditions outlined below.

# **Key Shared Parameters**

AVPhigh:	High end of Adjusted Vapor Pressure Range for the assessment (torr; 0 < AVPhigh; default AVPhigh = AVPhigh from <i>Preferences/Vapor Model Activation</i> )
AVPlow:	Low end of Adjusted Vapor Pressure Range for the assessment (torr; 0 < AVPlow; default AVPlow = AVPlow from <i>Preferences/Vapor Model Activation</i> )

AVPrm:	Adjusted Vapor Pressure for Raw Material for the selected operation (torr; 0 < AVPrm; read-only: AVPrm = Xrm x VP)
AVPprod:	Adjusted Vapor Pressure for Product for the selected operation (torr; 0 < AVPprod; read-only: AVPprod = Xprod x VP)
Xrm:	Vapor Pressure Correction Factor for Raw Material for the selected operation (dimensionless; 0 < Xrm < 1; default Xrm = Xprod for the PREVIOUS operation or, if no previous operation, 1)
Xprod:	Vapor Pressure Correction Factor for Product for the selected operation (dimensionless; 0 < Xprod < 1; default Xprod = Xrm)
Xother:	Vapor Pressure Correction Factor for Other Material for the selected operation (dimensionless; 0 < Xother < 1; default Xother = Xrm)

The Shared Parameters/Factors subtab will show the following parameters or factors. If a selected industry-specific operation has default models that share parameters or factors, those parameters or factors are shown in the Shared Parameters/Factors subtab (e.g., spray gun type for Automotive spray coating operations). These parameters will be preselected on the Shared Parameters/Factors subtab based on the operation except for the group of vapor model parameters, which may be preselected based on the following conditions. Industry operation shared parameters are described in the applicable industry-specific operation User Guide topic.

# Adjusted Vapor Pressure Range Default Values for the Current Assessment

The adjusted vapor pressure range (AVPlow and AVPhigh) for the current assessment is shown on this subtab. When a new assessment is started, the initial default values for this range are set to the values for the workstation on which ChemSTEER is being run. These workstation-specific values may be viewed and changed from the ChemSTEER menu item Preferences/<u>Vapor Model Activation</u>. You can change the values of this range by clicking on the value you wish to change and typing a new value.

If any AVP for the operation > AVPlow for the assessment, then the entire group of vapor model parameters (AVPrm, AVPprod, Xrm, Xprod, and Xother) are shown. Be sure to read the <u>Adjusted Vapor</u> <u>Pressure for the Operation</u> topic.

#### **Model Group Preselection Default Conditions**

You can change the availability of shared parameter/factor groups that were preselected by ChemSTEER by clicking the *Update Available Shared Parameters/Factors* button and manually selecting or deselecting model groups for each operation. Parameters or factors in the selected groups are displayed on the *Shared Parameters/Factors* subtab and are available for use by any model within that operation to which the parameter or factor applies. ChemSTEER may have default values (e.g., X=1) available to the models even if you have deselected the model group. ChemSTEER will retain the parameter defaults or user changes even after model groups have been deselected; however, you will need to select model groups to update values. When the user clicks on the *Update Available Shared Parameters/Factors* button on the *Shared Parameters/Factors* subtab, an update window will be displayed showing the selected shared parameter/factor groups and all shared parameter/factor groups that are available for the operation. The following shared parameters/factors groups are currently implemented in ChemSTEER:

- Vapor Pressure Shared Parameters (see <u>Adjusted Vapor Pressure for the Operation</u>)
- <u>Auto Spray Painting Shared Parameters</u>

The list of shared parameters on the *Shared Parameters/Factors* subtab will include the model group and the parameter/factor's name, type, value, and units. Depending on the parameter, the parameters may be updated by one of following methods after double clicking on the *Type* label of a particular parameter:

An update window will be launched to change the *Value* or *Type* label for that parameter or factor, or

You can change the *Type* label to either *Default* or *User-defined Default*. If you change the *Type* label to *User-defined Default*, the *Value* field for that specific shared parameter will become updateable. If you switch the shared parameter type back to *Default*, the value for that shared parameter will be reset to its default value.

# Adjusted Vapor Pressure for the Operation

An adjusted vapor pressure (AVP) for an operation is the product of a vapor pressure correction factor (X) for the material handled within the operation and the vapor pressure of the assessed chemical (VPchem). An AVP is used in determining whether vapor-related release and exposure models are appropriate default models for some liquid-related sources/ activities in an operation. For each operation, there are two AVP options: AVPrm and AVPprod.

The default adjusted vapor pressure (AVP) for each liquid-related source/ activity is determined as follows:

If the source/activity is for <u>product</u> (regardless of the operation type), then the default adjusted vapor pressure for the source/activity is **AVPprod**.

If the source/activity is for <u>raw material</u> (regardless of the operation type), then the default adjusted vapor pressure for the source/activity is **AVPrm**.

If the source/activity material is <u>unspecified</u> and it is used in a <u>manufacturing</u> operation, then the default adjusted vapor pressure for the source/activity is **AVPprod**.

Otherwise, the default adjusted vapor pressure for the source/activity is **AVPrm**.

You can change the value of an AVP for an operation by changing the vapor pressure correction factor (X) for that AVP. For example, AVPrm = Xrm x VP, so changing Xrm will change AVPrm. Instructions and options for changing values of X are discussed below.

# Default Model Selection Based on Adjusted Vapor Pressures

ChemSTEER selects default release models when you select an operation in the pull-down combo boxes in either the *Releases* or *Exposures* tabs. For each liquid source/activity for which ChemSTEER conditionally defaults to a vapor model, ChemSTEER compares the activity AVP to the adjusted vapor pressure range (see <u>Vapor Model Activation</u>) for the assessment.

If (*AVPlow* for the assessment) < (Default *AVP for the source/activity* (as specified in the indented paragraph above)) < (*AVPhigh* for the assessment),...

...then ChemSTEER will default to the specified vapor generation and mass balance inhalation models for the source/ activity.

Otherwise, ChemSTEER has no default model for vapor generation or vapor inhalation for the source/ activity.

If you change an AVP for the operation or the adjusted vapor pressure range for the assessment (i.e., AVPlow and/or AVPhigh) after the models have already been defaulted, ChemSTEER will determine whether the change would affect the current conditional defaulting. If the change results in a switch from being inside the range to outside or vice versa, ChemSTEER will display the following warning message:

"The default release and exposure models have already been defaulted for the previous AVP and Adjusted VP range, you may need to manually adjust your models based on the new VPchem, VP correction factor, or Adjusted VP range."

If you subsequently change the conditions so that neither of the operation's AVPs are greater than AVPlow, then the vapor model group (AVPrm, AVPprod, Xrm, Xprod, and Xother) will remain selected and visible in the *Shared Parameters/Factors* subtab; however, you can manually deselect groups of parameters on the *Shared Parameters/Factors* subtab.

# **Vapor Pressure Correction Factors**

Vapor pressure correction factors (X) are used in calculating adjusted vapor pressures for an operation as discussed above. These parameters are also inputs for vapor-related release and exposure models. The following general defaulting rules for X apply to most vapor-related models (see the specific model's Help topic for details on how X is used and on the available options for selecting X values in that model).

If the source/activity is for <u>product</u> (or the source/activity is not material specific and the operation is <u>manufacturing</u>), then the default X for the source/activity is **Xprod**.

Otherwise, the default X for the source/ activity is Xrm.

*Xother* gives you the option of calculating or specifying a third value of X for the operation.

Below is an explanation of options for calculating or specifying X values.

# **Key to Parameters and Abbreviations**

- a: Chemical or mixture designator for the operation (for any activities using raw material (rm), product (prod), or other user-defined material(other))
- jn: Designator for another chemical component in the mixture (limited to 5 total other components; n is integer where 1 < n < 5; j1 is for other chemical #1, ...)
- X: Vapor pressure correction factor for the chemical or other component in the mixture, dimensionless (0 < X < 1)
- Y: Weight fraction of the chemical or other component in the mixture, dimensionless (0 < Y < 1)
- MW: Molecular weight of chemical or other component in the mixture, positive number (0 < MW)

These parameters are used to perform calculations for vapor pressure correction factors for the chemical being assessed.

# Vapor Pressure Correction Factor Calculation

You can choose from the following four options to calculate the mole fraction calculation of Xrm, Xprod, and Xother (for Xother, assume Yrm for Ya):

- Xrm = Yprod from the previous operation or 1
- X = 1
- X = Ya (assume mole fraction approximates weight fraction)
- X = (Ya / MWa) / (Ya/MWa + Yj1/MWj1 + ...+ Yjn/MWjn) (mole fraction calculation using Raoult's Law)
- X = User-defined Default

# Auto Spray Painting Shared Parameters

When either the <u>Automobile OEM Spray Coating Application</u> operation or the <u>Automobile</u> <u>Refinish Spray Coating Application</u> operation is selected, the <u>Shared Parameters/Factors</u> subtab will display the Automotive Spray Painting shared parameters/factors, by default. You can change shared parameter default values by double-clicking on the desired parameter in the table. The default settings for each of these operations are summarized in the table below:

Shared Parameter/Factor	Default Setting For Automobile OEM Spray Coating	Default Setting for Automobile Refinish Spray Coating
Spray Gun Type	Conventional	Conventional
Overspray Control Type	Waterwash	Dry Filter
Booth Ventilation Type	Downdraft	Crossdraft

The combination of spray gun type and overspray control type determine the default calculations in either the <u>EPA/OPPT Automobile OEM Coating Overspray Loss Model</u> or the <u>EPA/OPPT</u> <u>Automobile Refinish Coating Overspray Loss Model</u>. Specifically it affects how the loss fraction of the coating is calculated, as well as the proportions that are released to air and other media.

The combination of spray gun type and booth ventilation type determine default calculations in either the EPA/OPPT Automobile OEM Spray Coating Inhalation Exposure Model or the EPA/OPPT Automobile Refinish Spray Coating Inhalation Exposure Model. These two default models estimate exposures to non-volatile non-polyisocyanate compounds in the coating mist. An alternative model for either the OEM or refinish operations is the EPA/OPPT Automobile Spray Coating Inhalation Exposure Model. This model can be used to calculate exposures to polyisocyanates. Specifically the shared parameters affect the default concentration of mist in the air used in calculating worker inhalation exposures.

# **ESTIMATING CHEMICAL RELEASES TAB**

You can use the *Estimating Chemical Releases* tab to view, update, and run the model(s) used to calculate the releases for each of the operations' sources/activities. In this tab you may view and/or update which models are used, view/update the specific model-related parameters, and view the model results (estimated releases).

# Changing the Model or Selecting Additional Models to Calculate a Release

For EACH Release Source/Activity of EACH OPERATION, you should first determine whether the Release Model(s) are those that you wish to use. If desired, change the selected model(s) by clicking the *Add or Remove a Release Model* button. Alternative models that are most applicable to the selected source/activity are listed in the *Available Models* box. To view ChemSTEER's entire collection of release models, click the *Show All Release Models* button.

Click on the model you wish to use for the selected source/activity to select it (the selected model is highlighted) and click the *Add to list* button. To remove a model, select it in the *Selected Models* box and click the *Remove from list* button. Click *OK* when you have finished choosing the models for the selected source/activity.

# Viewing and/or Updating a Model's Parameters

All parameters and settings used in the model are displayed in the *Release Input Parameters* subtab. Click the *View/Update Model Information* button to access an *Update* window for changing any parameter value that you wish to update. The selected model's equation(s) are displayed along with a list of all parameters and other settings. Additional details about the models, including the equations, logic, parameter options, and original references are available in the <u>ChemSTEER Estimation Methods</u> and <u>Models</u> section of the User Guide.

# Calculating Two Results With a Single Model

You may calculate two results from the same release model concurrently by enabling two sets of model input parameters. This function can be used to calculate alternative releases or a range in releases, depending on the nature of the differing input parameter values.

Some models have this capability enabled by default. To calculate a single result with these models, simply disable one of the sets of input parameters prior to running the model.

For additional details on how to use the dual-output model functions, read the <u>Calculating Two</u> <u>Sets of Results from a Single Model</u> topic.

# A Note About Vapor Generation Models

The following <u>vapor generation models</u> calculate parameters that are necessary to run a corresponding vapor inhalation model in the *Exposures* tab:

EPA/OAQPS AP-42 Loading Model EPA/OPPT Mass Transfer Coefficient Model EPA/OPPT Penetration Model User-Defined Vapor Generation Rate Model

In the unusual event that you wish to select more than one vapor generation model for a given Release Activity, you should assure that the model result to be used in a corresponding Exposure Activity vapor inhalation model is listed LAST on the *Release Model(s) for Selected Activity* list.

NOTE: If the adjusted vapor pressure (AVPrm or AVPprod) for the operation is less than the preferred AVPlow or greater than the preferred AVPhigh (be sure to review the <u>Operation Parameters</u> <u>Tab  $\rightarrow$  Shared Parameters/Factors Subtab</u> section of the User Guide), these vapor generation models will NOT be selected as defaults for any Release Activity within that operation. You must select these models manually.

# Modifying the Target Media of Release

You may change the medium/media of release by clicking on the *Modify Media of Release* button. The following receiving environmental media and alternative Media Sets (a Media Set has "or" between two or more environmental media) are available in ChemSTEER:

Water Water or Air Water or Incineration Water or Landfill Water or Air or Incineration Water or Air or Landfill Water or Incineration or Landfill Water or Air or Incineration or Landfill Air Air or Incineration Air or Landfill Air or Incineration or Landfill Incineration Incineration or Landfill Landfill Deepwell Injection Destroyed Other

Certain release models have pre-defined default media of release designations which depend on model input parameters. The models that include input parameters that affect the media of release are:

- EPA/OPPT Automobile OEM Coating Overspray Loss Model;
- EPA/OPPT Automobile Refinish Coating Overspray Loss Model;
- EPA/OPPT Electroplating Rinse Water Loss Model;
- <u>EPA/OPPT Electroplating Spent Bath Disposal Model</u>; and
- EPA/OPPT Solids Transfer Dust Loss Model.

If you make any changes to the media of release for these models and subsequently change input parameters, your media of release changes will be overwritten with default designations for the new input parameter(s). At the time you change default media of release for the models listed above, you will receive a warning. You may also refer to the Help section for each of these models.

# **Entering Introductory or Operation-Specific Notes for the Releases**

You may wish to record general information about the releases from an operation. One example of this general information includes, "Releases to water are not expected." In this example, it can be documented that, although releases are not expected from the operation, the reviewer did consider them. This text can be used to distinguish incomplete assessments from those in which all potential releases were considered.

This information can also be used to indicate whether multiple releases from the same operation to the same receiving medium are expected to occur on the same days or whether they occur on separate days.

Clicking the *Introductory Notes for the Release Summary* button displays a screen containing the following check boxes:

Add "Water: not expected"

Add "IRER Note: The daily releases listed for any source below may coincide with daily releases from the other sources to the same medium." [This note is the default for all operations]

Add "IRER Note: The daily releases listed for any source below are expected to coincide with daily releases from the other sources to the same medium."

Add "IRER Note: The daily releases listed for any source below are not expected to coincide with daily releases from the other sources to the same medium."

For each of the options that you check in this screen, the associated text is added to the text box. You also may modify the text in the box, as appropriate for the operation.

The information recorded in the Introductory Notes text box is included at the beginning of the ENVIRONMENTAL RELEASES ESTIMATE SUMMARY section the IRER report (see <u>IRER Format Details</u>). If no releases are calculated for the operation, this text will be the only item included in this section of the IRER.

# **Entering Additional Notes Pertaining to Releases of Related Chemicals**

Particular types of chemicals, by their nature, include additional releases beyond those that result directly from the operation (i.e., those that are calculated for each of the operation's release sources). For example, an assessment of a chemical compound containing a metal(s) may include release calculations for the amount of the chemical that is sent to an incinerator; however, the metallic components of the chemical are not destroyed by the incinerator. These components are typically deposited in the resulting ash, which may be subsequently sent to a landfill. Amounts of this ash may also be released to air through the stack.

These notes also allow EPA to assess particular compounds that could be formed as a result of the chemical's release and are of special concern. For example, EPA is currently examining the potential for compounds such as perfluorooctane sulfonate (PFOS) and perfluorooctanoic acid (PFOA) to be created from the release of other chemicals. ChemSTEER allows you to include an estimated quantity of these releases for use in assessing environmental and exposure risks.

These types of additional releases can be noted and included in the assessment by clicking the *Additional Notes for the Release Summary* button. ChemSTEER displays a screen containing the following default text:

"Perfluoro/Metal component/Hydrolysis product release to WATER or AIR or INCINERATION or LAND: kg/site-day over \* days/yr for \* sites or \* kg/yr to: from: basis: "

If you wish to note these types of releases from your operation in the IRER (see <u>IRER Format</u> <u>Details</u>), you **MUST** edit the above default text, as appropriate. You must click in the text box and click *OK* before the *Additional Notes* will appear at the end of the ENVIRONMENTAL RELEASES ESTIMATE SUMMARY section of the IRER.

# **Running the Models**

Click *Run Model(s)* and click on the *Estimated Releases* subtab to view model outputs. Repeat this process for each model used by the selected Release Activity. Repeat all steps for each Release Activity within each Operation of the assessment.

**NOTE:** Be aware that changing certain parameters in the *Chemical* tab and *Operation Parameters* subtabs will affect some of the parameter settings used in the release model estimates. Be sure to read about <u>Hierarchy of ChemSTEER Operations, Activities, and Models</u>.

# **Model Status Messages**

The following messages are displayed at the top of the *Release Input Parameters* subtab:

- *Model never run:* The selected model has not yet been run; results are not available.
- Model was successfully run: The selected model was run; results are available.
- **Model was unsuccessful:** The selected model attempted to run; however, was unsuccessful. This is usually the result of a missing parameter value. When the *Run Model(s)* button is clicked, ChemSTEER displays a message indicating which parameters were needed, but were unavailable. You must resolve the discrepancy in order to run the model and calculate results.
- *Model parms were changed, please re-run the models:* At least one parameter was changed since the model was last run; you must re-run the model in order to update the results.

# **ESTIMATING CHEMICAL EXPOSURES TAB**

You can use the *Estimating Chemical Exposures* tab to view, update, and run the model(s) used to calculate the dermal and/or inhalation exposures for each of the operations' activities. In this tab you may view and/or update which models are used, view/update the specific model-related parameters, and view the model results (estimated exposures). The Respirator Class and Monitoring Review subtab is read-only and the fields are described under the <u>IRER Format Details</u> topic.

# Changing the Model or Selecting Additional Models to Calculate an Exposure

For EACH Exposure Activity of EACH OPERATION, you should first determine whether the Exposure Model(s) are those that you want to use. If desired, change the selected model(s) by clicking the *Add or Remove a Release Model* button and choosing an alternative from either the *Dermal Model* and/or *Inhalation Model* combo boxes.

# Viewing and/or Updating a Model's Parameters

When a model you want to use is shown next to the Dermal Exposure or Inhalation Exposure Model label, you may view the parameters used in the model and, if needed, click the View/Update Model Information button to access an Update window for changing any parameter values that you wish to update.

All parameters and settings used in the dermal and inhalation exposure models are displayed in the *Dermal Model Input Parameters* and the *Inhalation Model Input Parameters* subtabs, respectively. Click the *View/Update Model Information* button to access an *Update* window for changing any parameter value that you wish to update. The selected model's equation(s) are displayed along with a list of all parameters and other settings. Additional details about the models, including the equations, logic, parameter options, and original references are available in the <u>ChemSTEER Estimation Methods</u> and <u>Models</u> section of the User Guide.

The Update window also contains an *Uncertainty* checkbox. This is primarily used by EPA reviewers and is an indication that there is some level of uncertainty associated with the inhalation exposure estimate included in the assessment (e.g., it is based a model, regulatory limit, or data that is

not specific to the industry). As a default, the *Uncertainty* is checked for each inhalation exposure estimate.

# Calculating Two Results With a Single Model

You may calculate two results from the same exposure model concurrently by enabling two sets of model input parameters. This function can be used to calculate alternative exposures or a range in exposures, depending on the nature of the differing input parameter values.

Some models have this capability enabled by default. To calculate a single result with these models, simply disable one of the sets of input parameters prior to running the model.

For additional details on how to use the dual-output model functions, read the <u>Calculating Two</u> <u>Sets of Results from a Single Model</u> topic.

# A Note About Vapor Inhalation Models

The following <u>vapor inhalation models</u> have input parameters that are determined from values set or calculated by corresponding vapor generation models in the *Releases* tab:

- EPA/OPPT Mass Balance Inhalation Model
- OSHA PEL-Limiting Model for Substance-Specific Vapors

In the unusual event that you select more than one vapor generation model for a given *Release* Activity in the Releases tab, you should assure that the model result to be used in the corresponding Exposure Activity vapor inhalation model is listed LAST on the *Release Model(s)* for Selected Activity list.

NOTE: If the adjusted vapor pressure (AVPrm or AVPprod) for the operation is less than the preferred AVPlow or greater than the preferred AVPhigh (be sure to review the <u>Operation Parameters</u> <u>Tab  $\rightarrow$  Shared Parameters/Factors Subtab</u> section), the vapor generation and vapor inhalation models will NOT be selected as defaults for any source/activity within that operation. You must select these models manually.

# Entering an Introductory or Operation-Specific Notes for the Inhalation Exposures

You may wish to record general information about the inhalation exposures in an operation. An example of this of this general information includes, "Inhalation is negligible (VP < 0.001 torr)". In this example, it can be documented that, although inhalation exposures are not expected in the operation, the reviewer did consider them. This text can be used to distinguish incomplete assessments from those in which all potential inhalation exposures were considered.

Clicking the *Introductory Notes for the Inhalation Summary* button in the *Inhalation Model Input Parameters* subtab displays a screen containing the following option in a drop-down box: "negligible (VP < 0.001 torr)".

When this option is selected, the text is added to the text box. You also may modify the text in the box, as appropriate for the operation.

The information that is recorded for the Introductory Notes text box is included in the OCCUPATIONAL EXPOSURES ESTIMATE SUMMARY – Inhalation section of the IRER report (see <u>IRER</u> <u>Format Details</u>). If no inhalation exposures are calculated for the operation, this text will be the only item included in this section of the IRER (any calculated dermal exposures will also be displayed in this section).

# Entering an Introductory or Operation-Specific Notes for the Dermal Exposures

You may wish to record general information about the dermal exposures in an operation. An example of this of this general information includes, "Dermal exposures are not assessed (corrosive chemical)". In this example, it can be documented that, although dermal exposures are not expected in the operation, the reviewer did consider them. This text can be used to distinguish incomplete assessments from those in which all potential dermal exposures were considered.

Clicking the *Introductory Notes for the Dermal Summary* button in the *Dermal Model Input Parameters* subtab displays a screen containing the following options in a drop-down box:

- Negligible Corrosives (pH > 12, pH < 2)
- Negligible Materials at temperatures > 140 F (60 C)
- Non-quantifiable (Some surface contact may occur if manually transferred) In cast solids (e.g., molded plastics) or in matrices (e.g., extruded pellets)
- Non-quantifiable "Dry" surface coatings (e.g., fiber spin finishes)
- Non-quantifiable Gases/vapors (some contact may occur in the absence of protective clothing)

When one of these options is selected, the text is added to the text box. You also may modify the text in the box, as appropriate for the operation.

The information that is recorded for the Introductory Notes text box is included in the OCCUPATIONAL EXPOSURES ESTIMATE SUMMARY – Dermal section of the IRER report (see <u>IRER Format</u> <u>Details</u>). If no inhalation exposures are calculated for the operation, this text will be the only item included in this section of the IRER (any calculated dermal exposures will also be displayed in this section).

# Update Operation Total Number of Workers Exposed Button

You may click the Update *Operation Total Number of Workers Exposed* button to view the update window containing an operation worker activity/exposures summary table. You may also change the default *Operation Total Number of Workers* estimated value that is calculated for the operation (default is the sum of each activity's total number of workers). Be sure to enter other information about the estimated total number of workers in the Basis box provided on this window.

NOTE: Each time you modify the operation's activities or run the exposure models, all values in the summary table will be updated, including the *Operation Total Number of Workers* estimated value if you entered an alternate number. Read below for additional details.

The following parameters are displayed on the update window:

Activity (read-only): Listing of activities with occupational exposure for the operation.

<u>Route (read-only)</u>: Route of exposure, inhalation and/or dermal, for the model(s) with the highest number of total workers for the activity.

Note: The following logic is used to determine the most appropriate route of exposure forming the basis for the total number of workers calculations:

- If there is the same *Activity total number of workers (NS x NWexp)* for inhalation and dermal, the Inhalation and Dermal will appear in the Route column.
- If there is the same Activity total number of workers (NS x NWexp) for inhalation and dermal, but the values for NS and NWexp are different, then Inhalation will appear in the Route column.
- If the Activity total number of workers (NS x NWexp) is greater for one route than the other, then only the route with the larger Activity total number of workers (NS x NWexp) will appear in the Route column.

<u>Number of sites (read-only)</u>: number of sites, NS, for the model(s) with the highest number of total workers for the activity.

<u>Number of workers per site (read-only)</u>: number of workers, NWexp, for the model(s) with the highest number of total workers for the activity.

<u>Activity total number of workers (read-only)</u>: product of the numbers of workers and sites (NS x NWexp) for the model(s) with the highest number of total workers for the activity.

Note: the Activity total number of workers (NS x NWexp) will be from the larger of Output 1 or Output 2.

<u>Operation total number of the workers default (sum from all activities) (read-only)</u>: sum of all products of the numbers of workers and sites (NS x NWexp) from the activities in the table.

<u>Operation total number of workers estimated:</u> initial default = sum of all products of the numbers of workers and sites (NS x NWexp) from the table. You may change this value to override the default.

If no model is run for an activity, all values in that row will display zeros. The *Operation total number of the workers default* will be recalculated when a new activity is added, when an activity is removed, when the exposure model Yes/No indicator on the *Sources/Activities* subtab is changed, and each time models are added, removed, or run for the operation. If the *Operation total number workers default* (sum from all activities) has changed, the *Operation total number of workers estimated* is reset to the default.

When the *Operation total number of workers estimated* has been reset, the *Basis* text will remain visible on the update window (for future use or reference) but will be grayed out (read-only) and will not appear on reports. You can restore the *Basis* text for reports

and modify by clicking on the *Operation total number of workers estimated* or by clicking on the *Basis* text.

# **Running the Models**

Click *Run Model(s)* and click on the *Estimated Releases* subtab to view model(s) outputs. Repeat this process for each model used by the selected Exposure Activity. Repeat all steps for each Exposure Activity within each Operation of the assessment.

NOTE: Be aware that changing certain parameters in the Chemical tab and Operation Parameters subtabs will affect some of the parameter settings used in the exposure model estimates. Be sure to read about <u>Hierarchy of ChemSTEER Operations, Activities, and Models</u>.

# **Model Status Messages**

The following messages are displayed at the top of the Dermal/Inhalation Model Input Parameters subtabs:

- *Model never run:* The selected model has not yet been run; results are not available.
- *Model was successfully run:* The selected model was run; results are available.
- **Model was unsuccessful:** The selected model attempted to run; however, was unsuccessful. This is usually the result of a missing parameter value. When the Run Model(s) button is clicked, ChemSTEER displays a message indicating which parameters were needed, but were unavailable. You must resolve the discrepancy in order to run the model and calculate results.
- *Model parms were changed, please re-run the models:* At least one parameter was changed since the model was last run; you must re-run the model in order to update the results.

# **OPTIONAL INFORMATION TAB**

The *Optional Information* tab allows the user to record EPA-related and other information, if applicable.

This tab contains several input screens that are each accessible by selecting a set of inputs from the combo box.

Some general, all-purpose information screens include:

- MSDS/Label/Exposure Limits this screen contains subtabs for recording MSDS requirements, relevant exposure limits, and LVE PPE (LVE PPE pertains to EPAassessments of Low Volume Exemption (LVE) submissions);
- Pollution Prevention Considerations; and
- Notes and Key Assumptions used in the assessment.

Some of the input screens are designed to serve EPA-related assessments, including:

- SAT Data;
- Exposure-based Criteria;

ChemSTEER may "double count" workers in select categories. For a single activity with dual outputs, 52 workers at 1.5 and 15 mg/day is considered 52 workers at 1-10 mg/day and 52 workers at >10 mg/day, while 52 workers at 2 and 6 mg/day is considered 52 workers at 1-10 mg/day.

- Physical State and Misc CRSS Info, Other uses, Occupational Exposure Rating, and Consumer Use (see additional information regarding the Occupational Exposure Rating below); and
- Special LVE Considerations.

# **Occupational Exposure Ratings (OERs)**

The Occupational Exposure Rating (OER) is an assessment-level read-only text box that is displayed when you select Physical State and Misc CRSS Info, Other Uses, Occupational Exposure Rating, and Consumer Use.

The OER is the combination of the *Numerical Ratings for Route and Dose* and the *Letter Ratings for Number of Workers*, as defined in the table below:

Rating	Criteria		
Numerical Ratings for Route and Dose			
NR	No occupational exposure assessment (e.g., low health concern). Inhalation and dermal routes not assessed per SAT.		
0-1	No exposure via routes assessed (=0 exposed workers). Each inhalation or dermal model estimate is 0 or has 0 workers, or there are no inhalation or dermal models but SAT requires inhalation or dermal assessments.		
1	Dermal only (no inhalation, i.e., no inhalation models or inhalation estimates are 0 and at least one dermal model is non-zero)		
1-2	Inhalation < 1 mg/day (considering each individual inhalation exposure)		
2	Inhalation 1-10 mg/day (considering each individual inhalation exposure)		
2-3	Inhalation > 10 mg/day (considering each individual inhalation exposure)		
Letter Ratings for Number of Workers			
А	<10 workers exposed for all assessed operations*		
В	<100 workers exposed for all assessed operations*		
С	<1000 workers exposed for all assessed operations*		
D	≥1000 workers exposed for all assessed operations*		

\* The total workers for the assessment is the sum of the *Operation total number of workers estimated* for all operations in the assessment. Go to the <u>Estimating Chemical Exposures Tab</u> topic of this User Guide (the *Update Operation Total Number of Workers Exposed* Button section) for more information.

Note that the exposure letter rating is not needed with numerical ratings associated with no exposure (i.e., NR and 0-1)). The highest possible numerical rating should be used when multiple criteria are met. For example, an assessment with dermal estimates, which produce a rating of 1, and inhalation estimates of both 0.5 mg/day, which produces a rating of 1-2, and 50 mg/day, which produces a rating

of 2-3, would be assigned a 2-3 rating (with the letter rating assigned based on the total number of workers estimated).

The OER is updated each time exposure models are run, when exposure models are added or removed (including when the exposure activity Yes/No indicator on the *Sources/Activities* tab is changed, when activities and operations are added or removed), and when you have specified the *total number of workers estimated*.

# **REPORTS TAB**

A reports tab has been included in the September 30, 2013 version of ChemSTEER to signify the end of the assessment process. These options are identical to those listed in the *File/ Reports* menu. View the <u>Generating and Viewing Summary Reports</u> section for a summary of options.

# Release Sources and Exposure Activities

In ChemSTEER, the term *Source/Activity* refers to sources and activities in an operation that can/do/will cause environmental releases and/or worker exposures. Most Sources/Activities have one or more default models that ChemSTEER uses to estimate releases and exposures. Choosing appropriate Sources/Activities allow you to access the models to make these estimates. Note: <u>you may include up to 20 sources/activities within each operation</u> included in the assessment.

Many industry-specific operations in ChemSTEER have preselected default Sources/Activities based on the sources and activities that are expected to occur in these operations. The user-defined operations require that you select the relevant Sources/Activities to assess.

Some Sources/Activities are specific to a particular industry (e.g., the Automotive Refinish Spray Coating Application source/activity), while other sources/activities are "broadly applicable" across many workplaces (e.g., the Loading Liquid Product into Drums or the Sampling Solid Raw Material sources/activities). The broadly applicable sources/activities available in ChemSTEER are only a subset of all possible sources and activities and cover those that are often overlooked or considered to be non-routine or insignificant.

When none of the other available Sources/Activities seem to cover a particular source/activity that you wish to assess, you may choose from the Sources/Activities listed under the *Miscellaneous Sources/Activities* category, which allow you the greatest flexibility in using ChemSTEER to estimate releases and/or exposures (i.e., these miscellaneous Sources/Activities allow you to choose the most appropriate release/exposure methods and models to use in the calculations).

Each selected Source/Activity activates one or more equations that represent methods and models that will quantify the release and/or exposure estimate(s). The Default Model Processing (DMP) status indicates whether each of the operation's selected sources/activities have been "processed" by ChemSTEER and have had their default models selected. The DMP status is displayed in the *Release DMP* and *Exposure DMP* columns of the *Sources/Activities* subtab of the *Operations* tab. Be sure to read more about ChemSTEER's hierarchy of functions, in particular the various DMP status indicators (click on the *Default Model Processing* link within <u>Hierarchy of ChemSTEER Operations</u>, Activities, and Models).

You can read more about the default methods and models, as well as the most appropriate alternatives, for each of the Sources/Activities by selecting one of the categories below to view the list of associated sources/activities. You may then select any of the sources/activities in the category list to view detailed information about that source/activity.

- Loading Liquids into Transport Containers/Vessels
- Loading Solids into Transport Containers/Vessels
- <u>Unloading Liquids from Transport Containers/Vessels</u>
- Unloading Solids from Transport Containers/Vessels
- <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>
- <u>Cleaning Solid Residuals from Transport Containers/Vessels</u>

- <u>Sampling Liquids</u>
- Sampling Solids
- Equipment Cleaning Losses of Liquids
- Equipment Cleaning Losses of Solids
- Unit Operations and Processes
- Vapor Release from Transfer Operations
- Miscellaneous Sources/Activities
- Automobile Spray Coating
- Generic Coating Applications
- <u>Electroplating Bath Additives</u>
- <u>Recirculating Water-Cooling Tower Additives</u>

# LOADING LIQUIDS INTO TRANSPORT CONTAINERS/VESSELS

# **Definition**

The loading of liquid product or raw material into transport containers/vessels that results in a release of the chemical and/or worker exposure to the chemical.

The following release sources/exposure activities may be selected for operations in which a liquid material containing the chemical is loaded into transport containers:

- Loading Liquid Product Into Bottles
- Loading Liquid Product Into Small Containers
- Loading Liquid Product Into Drums
- Loading Liquid Product Into Totes
- Loading Liquid Product Into Tank Trucks
- Loading Liquid Product Into Rail Cars
- Loading Liquid Product Into Containers
- Loading Liquid Raw Materials Into Containers
- Loading Liquid into Storage/Transport Vessels (User-defined)

The following table provides information on ChemSTEER default volumes and range of volumes for each type of container:

Vessel Name	Default Volume (Vc) [gal]	Range of Volumes [gal]
Loading Liquid Product Into Bottles	1	<5
Loading Liquid Product Into Small Containers	5	≥ 5 to < 20
Loading Liquid Product Into Drums	55	≥ 20 to < 100
Loading Liquid Product Into Totes	550	≥ 100 to < 1,000
Loading Liquid Product Into Tank Trucks	5,000	≥ 1,000 to < 10,000
Loading Liquid Product Into Rail Cars	20,000	≥ 10,000
Loading Liquid Product Into Containers	User-Defined	User-Defined
Loading Liquid into Storage/Transport Vessels (User-defined)	User-Defined	User-Defined

Source: portions from USEPA, 1991, Table 4-11.

For additional information on other container-specific parameters, go to <u>Container Parameters</u> <u>Guidance</u>.

# **Default Release**

The amount of chemical *released to air* from this source is calculated using the <u>EPA/OAQPS AP-</u> <u>42 Loading Model</u>.

**NOTE**: the air release model above is only defaulted if the selected operation's adjusted vapor pressure (AVPrm, AVPprod) is within the preferred range of AVPs. Refer to the <u>Operation</u> <u>Parameters Tab  $\rightarrow$  Shared Parameters/Factors Subtab</u> topic for more information. If the operation AVP is outside of the preferred range, there is no model for calculating releases to air from this source.

No default model exists for *releases to non-air media* from this source in ChemSTEER. OPPT assumes that releases from this source are insignificant when compared to other sources. If a release is expected, you must choose an appropriate model or specify a user-defined release to these media (see Other Release and Exposure Models, below).

# **Default Exposures**

Worker *inhalation* exposure to the chemical resulting from this activity is calculated using the <u>EPA/OPPT Mass Balance Inhalation Model</u>.

NOTE: the inhalation exposure model above is only defaulted if the selected operation's adjusted vapor pressure (AVPrm, AVPprod) is within the preferred range of AVPs. Refer to the <u>Operation Parameters Tab  $\rightarrow$  Shared Parameters/Factors Subtab</u> topic for more information. If the operation AVP is outside of the preferred range, there is no model for calculating worker inhalation exposures during this activity.

Worker *dermal* exposure to the chemical resulting from this activity is calculated using the <u>EPA/OPPT 2-Hand Dermal Contact with Liquid Model</u>.

# **Other Release and Exposure Models**

The default release and exposure models assume that the most significant release and exposure during the loading operation is from the displacement of air containing chemical vapor as a container/vessel is filled with liquid. You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur during loading of liquid product into bottles. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following alternative models may be used to estimate releases that occur from this source. These models may also be selected *in addition* to the default, as appropriate.

- User-Defined Loss Rate Model
- User-Defined Vapor Generation Rate Model

The following alternative inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- OSHA PEL-Limiting Model for Substance-Specific Vapors
- User-Defined Inhalation Model

The following alternative dermal exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

• EPA/OPPT 1-Hand Dermal Contact with Liquid Model

<u>US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.</u>

• User-Defined Dermal Model

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

# **UNLOADING LIQUIDS FROM TRANSPORT CONTAINERS/VESSELS**

# **Definition**

The unloading of liquid product or raw material from transport containers/vessels that results in a release of the chemical and/or worker exposure to the chemical.

The following release sources/exposure activities may be selected for operations in which a liquid material containing the chemical is loaded into transport containers:

- Unloading Liquid Raw Material from Bottles
- Unloading Liquid Raw Material from Small Containers
- Unloading Liquid Raw Material from Drums

- Unloading Liquid Raw Material from Totes
- Unloading Liquid Raw Material from Tank Trucks
- Unloading Liquid Raw Material from Rail Cars
- Unloading Liquid Raw Material from Containers
- Unloading Liquid Product from Containers
- Unloading Liquid from Storage/Transport Vessels (User-defined)

The following table provides information on ChemSTEER default volumes and range of volumes for each type of container:

Vessel Name	Default Volume (Vc) [gal]	Range of Volumes [gal]
Unloading Liquid Raw Material from Bottles	1	<5
Unloading Liquid Raw Material from Small Containers	5	≥ 5 to < 20
Unloading Liquid Raw Material from Drums	55	≥ 20 to < 100
Unloading Liquid Raw Material from Totes	550	≥ 100 to < 1,000
Unloading Liquid Raw Material from Tank Trucks	5,000	≥ 1,000 to < 10,000
Unloading Liquid Raw Material from Rail Cars	20,000	≥ 10,000
Unloading Liquid Product Into Containers	User-Defined	User-Defined
Unloading Liquid into Storage/Transport Vessels (User-defined)	User-Defined	User-Defined
Source: portions from LISERA 1991 Table 4-11		

Source: portions from USEPA, 1991, Table 4-11.

For additional information on other container-specific parameters, go to <u>Container Parameters</u> <u>Guidance</u>.

# **Default Release**

The <u>EPA/OAQPS AP-42 Loading Model</u> is the default for calculating releases of the chemical *to air* during unloading. It is assumed that as the container is unloading, another is being loaded. The default model provides a more conservative estimate of chemical releases that occur during this activity.

**NOTE**: the air release model above is only defaulted if the selected operation's adjusted vapor pressure (AVPrm, AVPprod) is within the preferred range of AVPs. Refer to the <u>Operation</u> <u>Parameters Tab  $\rightarrow$  Shared Parameters/Factors Subtab</u> topic for more information. If the operation AVP is outside of the preferred range, there is no model for calculating releases to air from this source.

No default model exists for *releases to non-air media* from this source in ChemSTEER. OPPT assumes that releases from this source are insignificant when compared to other sources. If a release is expected, you must choose an appropriate model or specify a user-defined release to these media (see *Other Release and Exposure Models*, below).

# **Default Exposures**

Worker *inhalation* exposure to the chemical resulting from this activity is calculated using the <u>EPA/OPPT Mass Balance Inhalation Model</u>

**NOTE**: the inhalation exposure model above is only defaulted if the selected operation's adjusted vapor pressure (AVPrm, AVPprod) is within the preferred range of AVPs. Refer to the <u>Operation Parameters Tab  $\rightarrow$  Shared Parameters/Factors Subtab</u> topic for more information. If the operation AVP is outside of the preferred range, there is no model for calculating worker inhalation exposures during this activity.

Worker *dermal* exposure to the chemical resulting from this activity is calculated using the <u>EPA/OPPT 2-Hand Dermal Contact with Liquid Model</u>

# **Other Release and Exposure Models**

The default release and exposure models assume that the most significant release and exposure during the unloading operation is from the displacement of air containing chemical vapor as another container/vessel is filled with liquid. You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur during unloading of liquid raw material from bottles. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following alternative models may be used to estimate releases that occur from this source. These models may also be selected *in addition* to the default, as appropriate.

- <u>EPA/OPPT Penetration Model</u> (for indoor activities, air speed is ≤ 100 feet/min)
- <u>EPA/OPPT Mass Transfer Coefficient Model</u> (for outdoor activities; air speed >100 feet/min)
- User-Defined Loss Rate Model
- User-Defined Vapor Generation Rate Model

The following alternative inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- OSHA PEL-Limiting Model for Substance-Specific Vapors
- User-Defined Inhalation Model

The following alternative dermal exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

• EPA/OPPT 1-Hand Dermal Contact with Liquid Model

US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.

EPA/OPPT 2-Hand Dermal Immersion with Liquid Model

<u>US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal</u> <u>Exposure, September 2013.</u>

• User-Defined Dermal Model

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

# LOADING SOLIDS INTO TRANSPORT CONTAINERS/VESSELS

# **Definition**

The loading of solid raw material or product material into transport containers that results in a release of the chemical and/or worker exposure to the chemical.

The following release sources/exposure activities may be selected for operations in which a solid material containing the chemical is loaded into transport containers:

- Loading Solid Product into Transport Containers
- Loading Solid Raw Materials into Transport Containers
- Loading Solids into Storage/Transport Vessels (User-defined)

The following table provides information on ChemSTEER default volumes and range of volumes for each type of container:

Vessel Name	Default Volume (Vc) [gal]	Range of Volumes [gal]
Loading Solid Product into Transport Containers		
Loading Solid Raw Material into Transport Containers	User-Defined	None
Loading Solids into Storage/Transport Vessels (User-defined)		

For additional information on container-specific parameters, go to <u>Container Parameters</u> <u>Guidance</u>.

# **Default Release**

Multi-media Release: The amount of chemical released to both air and non-air media as a result of dust generated by this activity is calculated using the <u>EPA/OPPT Solids Transfer Dust Loss Model</u>. This model apportions amounts of the dust collected to various media, determined by the control technology (if applicable).

# **Default Exposures**

Worker *inhalation* exposure to the chemical resulting from this activity is calculated using one of the following models:

• If the amount of product packaged per site-day (i.e., MCi x Ncd in the Container Parameters subtab of the Operation Parameters tab) < 54 kg/site-day, then the EPA/OPPT Small Volume Solids Handling Inhalation Model is used as a default.

• If the amount of product packaged per site-day > 54 kg/site-day, then either the <u>OSHA</u> <u>Respirable PNOR PEL-Limiting Model</u> or <u>OSHA Total PNOR PEL-Limiting Model</u> may be chosen as a default.

NOTE: If the daily amount of material loaded was not calculated by ChemSTEER before the inhalation exposure is calculated, the daily amount of material throughput from the Mass Balance calculations will be used.

If the throughput was not calculated, the <u>OSHA Total PNOR PEL-Limiting Model</u> will be used as a default.

Worker dermal exposure to the chemical resulting from this activity is calculated using the <u>EPA/OPPT Direct 2-Hand Dermal Contact with Solids Model</u>.

# Other Release and Exposure Models

The default exposure models assume that the most significant exposure during the loading operation is from the generation of dusts containing chemical as a container/vessel is filled with solids. You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur during loading of solid product into containers. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following model may be used to estimate releases that occur from this source. More than one release model may be used at one time to estimate releases, as appropriate.

User-Defined Loss Rate Model

The following alternative inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- OSHA PEL-Limiting Model for Substance-Specific Particulates
- User-Defined Inhalation Model

The following alternative dermal exposure model may be used to estimate the worker exposure that occurs as a result of performing this activity:

US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.

User-Defined Dermal Model

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

# **UNLOADING SOLIDS FROM TRANSPORT CONTAINERS/VESSELS**

# **Definition**

The unloading of solid raw material or product material into transport containers that results in a release of the chemical and/or worker exposure to the chemical.

The following release sources/exposure activities may be selected for operations in which a solid material containing the chemical is unloaded from transport containers:

- Unloading Solid Raw Materials from Transport Containers
- Unloading Solid Product from Transport Containers
- Unloading Solids from Storage/Transport Vessels (User-defined)

The following table provides information on ChemSTEER default volumes and range of volumes for each type of container:

Vessel Name	Default Volume (Vc) [gal]	Range of Volumes [gal]
Unloading Solid Raw Material from Transport Containers		
Unloading Solid Product from Transport Containers	User-Defined	None
Unloading Solids from Storage/Transport Vessels (User-defined)		

For additional information on container-specific parameters, go to <u>Container Parameters</u> <u>Guidance</u>

# Default Release

Multi-media Release: The amount of chemical released to both air and non-air media as a result of dust generated by this activity is calculated using the <u>EPA/OPPT Solids Transfer Dust Loss Model</u>. This model apportions amounts of the dust collected to various media, determined by the control technology (if applicable).

# **Default Exposures**

Worker *inhalation* exposure to the chemical resulting from this activity is calculated using one of the following models:

- If the amount of raw material unloaded per site-day (i.e., MCi x Ncd in the *Container Parameters* subtab of the *Operation Parameters* tab) < 54 kg/site-day, then the <u>EPA/OPPT Small Volume Solids Handling Inhalation Model</u> is used as a default.
- If the amount of raw material unloaded per site-day > 54 kg/site-day, then either the <u>OSHA Total PNOR PEL-Limiting Model</u> or <u>OSHA Respirable PNOR PEL-Limiting Model</u> may be chosen as a default.

NOTE: If the daily amount of material unloaded was not calculated by ChemSTEER before the inhalation exposure is calculated, the daily amount of material throughput from the Mass Balance calculations will be used.

If the throughput was not calculated, the <u>OSHA Total PNOR PEL-Limiting Model</u> will be used as a default.

Worker *dermal* exposure to the chemical resulting from this activity is calculated using the <u>EPA/OPPT Direct 2-Hand Dermal Contact with Solids Model</u>.

# **Other Release and Exposure Models**

The default exposure models assume that the most significant exposure during the unloading operation is from the generation of dusts containing chemical as a container/vessel containing solids is emptied. You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur during unloading of solid raw material from containers. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following model may be used to estimate releases that occur from this source. More than one release model may be used at one time to estimate releases, as appropriate.

• User-Defined Loss Rate Model

The following alternative inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- OSHA PEL-Limiting Model for Substance-Specific Particulates
- User-Defined Inhalation Model

The following alternative dermal exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

• EPA/OPPT 2-Hand Dermal Contact with Container Surfaces Model

US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.

User-Defined Dermal Model

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

# **CLEANING LIQUID RESIDUALS FROM TRANSPORT CONTAINERS/VESSELS**

# **Definition**

The cleaning of raw material or product residues from "empty" transport containers/vessels with a liquid cleaning medium that results in a release of the chemical and/or worker exposure to the

chemical. This release source/worker activity is also relevant to the disposal of liquid residues with the empty container/vessel.

The following release sources/exposure activities may be selected for operations in which a liquid material containing the chemical is cleaned from or disposed with "empty" transport containers:

Activities for Raw Materials and Products:

- Cleaning Liquid Residuals from Bottles Used to Transport the Raw Material/Product
- Cleaning Liquid Residuals from Small Containers Used to Transport the Raw Material/Product
- Cleaning Liquid Residuals from Drums Used to Transport the Raw Material/Product
- Cleaning Liquid Residuals from Totes Used to Transport the Raw Material/Product
- Cleaning Liquid Residuals from Tank Trucks Used to Transport the Raw Material/Product
- Cleaning Liquid Residuals from Rail Cars Used to Transport the Raw Material/Product
- Cleaning Liquid Residuals from Containers Used to Transport the Raw Material/Product
- Cleaning Liquid Residuals from Storage/Transport Vessels (User-defined)

The following table provides information on ChemSTEER default volumes and range of volumes for each type of container:

Vessel Name	Default Volume (Vc) [gal]	Range of Volumes [gal]
Unloading Liquid Raw Material from Bottles	1	<5
Unloading Liquid Raw Material from Small Containers	5	≥ 5 to < 20
Unloading Liquid Raw Material from Drums	55	≥ 20 to < 100
Unloading Liquid Raw Material from Totes	550	≥ 100 to < 1,000
Unloading Liquid Raw Material from Tank Trucks	5,000	≥ 1,000 to < 10,000
Unloading Liquid Raw Material from Rail Cars	20,000	≥ 10,000
Unloading Liquid Product Into Containers	User-Defined	User-Defined
Unloading Liquid into Storage/Transport Vessels (User-defined)	User-Defined	User-Defined

Source: portions from USEPA, 1991, Table 4-11.

For additional information on other container-specific parameters, go to <u>Container Parameters</u> <u>Guidance</u>.

# **Default Releases**

# Air Release:

It is assumed that cleaning activities for bottles, small containers, drums, and totes are performed indoors (i.e., air speed is  $\leq$  100 feet/min). The amount of chemical release from these sources is thus calculated using the <u>EPA/OPPT Penetration Model</u>.
For tank trucks and rail cars, it is assumed that the cleaning activities are performed outdoors (i.e., air speed is > 100 feet/min). The amount of chemical release from this source is thus calculated using the <u>EPA/OPPT Mass Transfer Coefficient Model</u>.

NOTE: the air release models above are only defaulted if the selected operation's adjusted vapor pressure (AVPrm, AVPprod) is within the preferred range of AVPs. Refer to the <u>Operation</u> <u>Parameters Tab  $\rightarrow$  Shared Parameters/Factors Subtab</u> topic for more information. If the operation AVP is outside of the preferred range, there is no model for calculating releases to air from this source.

Non-Air Release:

Release of the residual raw material/product in the "empty" container is calculated using the either the <u>EPA/OPPT Small Container Residual Model</u>, <u>EPA/OPPT Drum Residual Model</u>, or <u>EPA/OPPT Bulk Transport Residual Model</u>, depending on the container size.

The following table summarizes the default air and non-air release models for each type of container:

Vessel Name	Default Air Release Models	Default Non-Air Release Models
Bottles	EPA/OPPT Penetration Model	EPA/OPPT Small Container Residual Model
Small Containers		
Drums		EPA/OPPT Drum Residual Model
Totes		
Tank Truck	EDA (ODDT Massa Turanafan Calaffiniant Madal	EPA/OPPT Bulk Transport Residual Model
Rail Car		
Containers	No default model - If a release to air is expected, you must choose an appropriate model or specify a user-defined release to air (see Other Release and Exposure Models, below).	EPA/OPPT Drum Residual Model
Storage/Transport Vessels (User- Defined)	EPA/OPPT Penetration Model	EPA/OPPT Drum Residual Model

## Default Exposures

Worker *inhalation* exposure to the chemical resulting from these activities is calculated using the <u>EPA/OPPT Mass Balance Inhalation Model</u>.

**NOTE**: In order to utilize the above vapor inhalation model, you must select and run a vapor generation release model for this source/activity in order to obtain the necessary input parameters for this model.

NOTE: the inhalation exposure model above is only defaulted if the selected operation's adjusted vapor pressure (AVPrm, AVPprod) is within the preferred range of AVPs. Refer to the <u>Operation Parameters Tab  $\rightarrow$  Shared Parameters/Factors Subtab</u> topic for more information. If

the operation AVP is outside of the preferred range, there is no model for calculating worker inhalation exposures during this activity.

Worker *dermal* exposure to the chemical resulting from these activities is calculated using the <u>EPA/OPPT 2-Hand Dermal Contact with Liquid Model</u>.

The following table summarizes the default inhalation and dermal exposure models for each type of container:

Vessel Name	Default Inhalation Exposure Models	Default Dermal Exposure Models
Bottles	<u>EPA/OPPT Mass Balance Inhalation Model</u>	<u>EPA/OPPT 2-Hand Dermal Contact with</u> Liquid Model
Small Containers		
Drums		
Totes		
Tank Truck		
Rail Car		
Containers		
Storage/Transport Vessels (User- Defined)		

### **Other Release and Exposure Models**

The default release and exposure models assume that the most significant release and exposure during the cleaning operation is from disposal of liquid residues containing the chemical and from the evaporation of volatile liquid residues containing chemical vapor. You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur during cleaning and disposal of liquid bottle residues. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following table presents alternative models may be used to estimate releases that occur from this source. These models may also be selected *in addition* to the default, as appropriate.

Vessel Name	Other Release Models
Bottles	EPA/OPPT Mass Transfer Coefficient Model (for outdoor activities; air speed >100 feet/min)
Small Containers	EPA/OAQPS AP-42 Loading Model
	EPA/OPPT Drum Residual Model
Totes	User-Defined Loss Rate Model
	User-Defined Vapor Generation Rate Model
Drums	EPA/OPPT Mass Transfer Coefficient Model (for outdoor activities; air speed >100 feet/min)
	EPA/OAQPS AP-42 Loading Model
Storage/Transport Vessels (User-Defined)	User-Defined Loss Rate Model
	User-Defined Vapor Generation Rate Model
Tank Truck	EPA/OPPT Penetration Model (for indoor activities; air speed ≤100
Rail Car	feet/min)
	EPA/OAQPS AP-42 Loading Model
	User-Defined Loss Rate Model
	User-Defined Vapor Generation Rate Model
Containers	EPA/OPPT Penetration Model (for indoor activities; air speed ≤100 feet/min)
	<u>EPA/OPPT Mass Transfer Coefficient Model</u> (for outdoor activities; air speed >100 feet/min)
	EPA/OAQPS AP-42 Loading Model
	EPA/OPPT Small Container Residual Model
	EPA/OPPT Bulk Transport Residual Model
	User-Defined Loss Rate Model
	User-Defined Vapor Generation Rate Model

The following alternative inhalation and dermal exposure models may be used to estimate the worker exposure that occurs as a result of performing these activities:

Vessel Name	Other Inhalation Exposure Models	Other Dermal Exposure Models
Bottles		EPA/OPPT 1-Hand Dermal Contact with
Small Containers		Liquid Model
Drums		US EPA Memo entitled Updating
Totes		CEB's Method for Screening-
Tank Truck	OSHA PEL-Limiting Model for Substance-	Exposure. September 2013.
Rail Car	Specific Vapors	EPA/OPPT 2-Hand Dermal Immersion
Containers	User-Defined Inhalation Model	with Liquid Model
Storage/Transport Vessels (User-Defined)		US EPA Memo entitled Updating CEB's Method for Screening-
		Level Assessments of Dermal
		Exposure, September 2013. User-Defined Dermal Model

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

# **CLEANING SOLID RESIDUALS FROM TRANSPORT CONTAINERS/VESSELS**

## **Definition**

The cleaning of solid raw material or product residues from "empty" containers that results in a release of the chemical and/or worker exposure to the chemical. This release source/worker activity is also relevant to the disposal of solid residues with the empty container.

The following release sources/exposure activities may be selected for operations in which a solid material containing the chemical is cleaned from or disposed with "empty" transport containers:

- Cleaning Solid/Powder Residuals from Container Used to Transport the Raw Material
- Cleaning Solid/Powder Residuals from Container Used to Transport the Product
- Cleaning Solid/Powder Residuals from Storage/Transport Vessels (User-defined)

For additional information on container-specific parameters, go to <u>Container Parameters</u> <u>Guidance</u>.

### **Default Releases**

Release of the residual raw material to *non-air media* from the "empty" container is calculated using the <u>EPA/OPPT Solid Residuals in Transport Containers Model</u>.

No default model exists for releases to air from these sources in ChemSTEER. If a release to air is expected, you must choose an appropriate model or specify a user-defined release to air (see *Other Release and Exposure Models*, below).

### **Default Exposures**

Worker *inhalation* exposure to the chemical resulting from this activity is calculated using one of the following models:

- If the daily amount of raw material in the containers (i.e., MCi x Ncd in the *Container Parameters* subtab of the *Operation Parameters* tab) < 54 kg/site-day, then the <u>EPA/OPPT Small Volume Solids Handling Inhalation Model</u> is used as a default.
- If the daily amount of raw material in the containers > 54 kg/site-day, then either the <u>OSHA Total PNOR PEL-Limiting Model</u> or <u>OSHA Respirable PNOR PEL-Limiting Model</u> may be chosen as a default.

**NOTE**: If the daily amount of raw material in the containers was not calculated by ChemSTEER before the inhalation exposure is calculated, the daily amount of material throughput from the Mass Balance calculations will be used.

If the throughput was not calculated, the <u>OSHA Total PNOR PEL-Limiting Model</u> will be used as a default.

EPA Assessment Policy Recommendation: It is recommended that the <u>amount of solid residue</u> that is cleaned from or disposed with the emptied container (i.e., the loss fraction x MCi x Ncd) be used to select the default inhalation model, instead using the total amount in the container before it is emptied (MCi x Ncd), as described above.

Worker *dermal* exposure to the chemical resulting from this activity is calculated using the <u>EPA/OPPT Direct 2-Hand Dermal Contact with Solids Model</u>.

### **Other Release and Exposure Models**

The default release and exposure models assume that the most significant release and exposure during the cleaning operation is from disposal of solid residues containing the chemical and from the generation of dust containing chemical. You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur during cleaning and disposal of solid raw material container residues. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following alternative model may be used to estimate releases that occur from this source. The model may also be selected *in addition* to the default, as appropriate.

User-Defined Loss Rate Model

The following alternative inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- OSHA PEL-Limiting Model for Substance-Specific Particulates
- User-Defined Inhalation Model

The following alternative dermal exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

• EPA/OPPT 2-Hand Dermal Contact with Container Surfaces Model

US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.

User-Defined Dermal Model

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

# **SAMPLING LIQUIDS**

## **Definition**

The sampling of liquids that results in a release of the chemical and/or worker exposure to the chemical.

The following release sources/exposure activities may be selected for operations in which a liquid material containing the chemical is sampled:

- Sampling Liquid Raw Material
- Sampling Liquid Product
- Sampling Liquids

## **Default Releases**

It is assumed that these activities are performed indoors (i.e., air speed is  $\leq$  100 feet/min) and the <u>EPA/OPPT Penetration Model</u> is used as a default for *releases to air*.

NOTE: the air release model above is only defaulted if the selected operation's adjusted vapor pressure (AVPrm, AVPprod) is within the preferred range of AVPs. Refer to the <u>Operation</u> <u>Parameters Tab  $\rightarrow$  Shared Parameters/Factors Subtab</u> topic for more information. If the operation AVP is outside of the preferred range, there is no model for calculating releases to air from this source.

No default model exists for releases to *non-air media* from these sources in ChemSTEER. OPPT assumes that releases from these sources are insignificant when compared to other sources. If a release is expected, you must choose an appropriate model or specify a user-defined release to these media (see *Other Release and Exposure Models*, below).

## **Default Exposures**

Worker *inhalation* exposure to the chemical resulting from these activities is calculated using the <u>EPA/OPPT Mass Balance Inhalation Model</u>.

**NOTE:** the inhalation exposure model above is only defaulted if the selected operation's adjusted vapor pressure (AVPrm, AVPprod) is within the preferred range of AVPs. Refer to the <u>Operation Parameters Tab  $\rightarrow$  Shared Parameters/Factors Subtab</u> topic for more information. If the operation AVP is outside of the preferred range, there is no model for calculating worker inhalation exposures during this activity.

Worker *dermal* exposure to the chemical resulting from these activities is calculated using the <u>EPA/OPPT 1-Hand Dermal Contact with Liquid Model</u>.

## **Other Release and Exposure Models**

The default release and exposure models assume that the most significant release and exposure during the sampling operation is from the evaporation of volatile liquid containing chemical vapor from open surfaces. You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur during sampling of liquids. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following alternative models may be used to estimate releases that occur from this source. These models may also be selected *in addition* to the default, as appropriate.

- <u>EPA/OPPT Mass Transfer Coefficient Model</u> (for outdoor activities; air speed >100 feet/min)
- User-Defined Loss Rate Model
- <u>User-Defined Vapor Generation Rate Model</u>

The following alternative inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- OSHA PEL-Limiting Model for Substance-Specific Vapors
- User-Defined Inhalation Model

The following alternative dermal exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

• EPA/OPPT 2-Hand Dermal Contact with Liquid Model

<u>US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal</u> <u>Exposure, September 2013.</u>

EPA/OPPT 2-Hand Dermal Immersion with Liquid Model

<u>US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal</u> <u>Exposure, September 2013.</u>

User-Defined Dermal Model

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

# **SAMPLING SOLIDS**

### **Definition**

The sampling of solid raw material or product that results in a release of the chemical and/or worker exposure to the chemical.

The following release sources/exposure activities may be selected for operations in which a solid material containing the chemical is sampled:

- Sampling Solid Raw Material
- Sampling Solid Product
- Sampling Solids

### **Default Release**

No default model exists for releases to the environment from these sources in ChemSTEER. OPPT assumes that releases from this source are insignificant when compared to other sources. If a release is expected, you must choose an appropriate model or specify a user-defined release (see *Other Release and Exposure Models*, below).

### **Default Exposures**

Worker *inhalation* exposure to the chemical resulting from these activities is calculated using the <u>EPA/OPPT Small Volume Solids Handling Inhalation Model</u>.

Worker *dermal* exposure to the chemical resulting from these activities is calculated using the EPA/OPPT Direct 2-Hand Dermal Contact with Solids Model.

### **Other Release and Exposure Models**

The default exposure models assume that the most significant exposure during the sampling operation is from handling solid materials containing chemical. You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur during unloading of solid raw material from containers. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following model may be used to estimate releases that occur from this source. More than one release model may be used at one time to estimate releases, as appropriate.

User-Defined Loss Rate Model

The following alternative inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing these activities:

- OSHA PEL-Limiting Model for Substance-Specific Particulates
- OSHA Total PNOR PEL-Limiting Model
- OSHA Respirable PNOR PEL-Limiting Model
- User-Defined Inhalation Model

The following alternative dermal exposure models may be used to estimate the worker exposure that occurs as a result of performing these activities

• EPA/OPPT 2-Hand Dermal Contact with Container Surfaces Model

US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.

User-Defined Dermal Model

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

# **EQUIPMENT CLEANING LOSSES OF LIQUIDS**

## **Definition**

The cleaning of product residues from one or more process vessels with a liquid cleaning medium that results in a release of the chemical and/or worker exposure to the chemical.

The following release sources/exposure activities may be selected for operations in which a liquid washout is performed on process equipment containing chemical:

- Equipment Cleaning Losses from a Single, Small Vessel
- Equipment Cleaning Losses from a Single, Large Vessel
- Equipment Cleaning Losses from Multiple Vessels

### **Default Releases**

*Air Release:* It is assumed that this activity is performed outdoors (i.e., air speed is >100 feet/min). The amount of chemical release from this source is thus calculated using the EPA/OPPT Mass Transfer Coefficient Model.

**NOTE:** the air release model above is only defaulted if the selected operation's adjusted vapor (AVPrm, AVPprod) is within the preferred range of AVPs. Refer to the <u>Operation Parameters Tab</u>

 $\rightarrow$  Shared Parameters/Factors Subtab topic for more information. If the operation AVP is outside of the preferred range, there is no model for calculating releases to air from this source.

*Non-Air Release:* Release of the residual product contained in the single process vessel is calculated using either the <u>EPA/OPPT Single Vessel Residual Model</u> or <u>EPA/OPPT Multiple Process Vessel</u> <u>Residual Model</u>, as specified below:

Equipment Cleaning Source	Default Non-Air Release	
Equipment Cleaning Losses from a Single, Small Vessel	EDA (ODDT Single Massel Residual Madel	
Equipment Cleaning Losses from a Single, Large Vessel	EPA/OPPT SINgle Vesser Residual Model	
Equipment Cleaning Losses from Multiple Vessels	EPA/OPPT Multiple Process Vessel Residual Model	

### **Default Exposures**

No default model exists for worker exposures during this activity in ChemSTEER. OPPT assumes that equipment cleaning is automated and that exposures during this activity are insignificant when compared to other activities. If exposures are expected, you must choose an appropriate model or specify a user-defined exposure (see *Other Release and Exposure Models*, below).

## Other Release and Exposure Models

The default release models assume that the most significant release during the cleaning operation is from disposal of liquid residues containing the chemical and from the evaporation of volatile liquid residues containing chemical vapor. You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur during the cleaning of a single process vessel. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following alternative models may be used to estimate releases that occur from this source. These models may also be selected *in addition* to the default, as appropriate.

- <u>EPA/OPPT Penetration Model</u> (for indoor activities; air speed ≤ 100 feet/min)
- EPA/OAQPS AP-42 Loading Model
- <u>EPA/OPPT Multiple Process Vessel Residual Model</u> (for Equipment Cleaning Losses from Single, Small Vessel or Equipment Cleaning Losses from Single, Large Vessel)
- User-Defined Loss Rate Model
- <u>User-Defined Vapor Generation Rate Model</u>

The following inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- EPA/OPPT Mass Balance Inhalation Model
- OSHA PEL-Limiting Model for Substance-Specific Vapors
- User-Defined Inhalation Model

The following dermal exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- EPA/OPPT 1-Hand Dermal Contact with Liquid Model
- EPA/OPPT 2-Hand Dermal Contact with Liquid Model

<u>US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal</u> <u>Exposure, September 2013.</u>

• EPA/OPPT 2-Hand Dermal Immersion with Liquid Model

<u>US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal</u> <u>Exposure, September 2013.</u>

User-Defined Dermal Model

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

# **EQUIPMENT CLEANING LOSSES OF SOLIDS**

The following release source/exposure activity may be selected for operations in which a solid residue containing the chemical is cleaned from process equipment:

Equipment Cleaning Losses of Solids from Process Vessels

## Equipment Cleaning Losses of Solids from Process Vessels

## **Definition**

The cleaning of solid product residues from process vessels that results in a release of the chemical and/or worker exposure to the chemical.

## **Default Releases**

Release of the residual solid product to *non-air media* from the process vessels is calculated using the <u>EPA/OPPT Solid Residuals in Transport Containers Model</u>.

No default model exists for *releases to air* from this source in ChemSTEER. If a release to air is expected, you must choose an appropriate model or specify a user-defined release to these media (see *Other Release and Exposure Models*, below).

### **Default Exposures**

Worker *inhalation* exposure to the chemical resulting from this activity is calculated using one of the following models:

For *continuous* operations:

- If the daily mass of product output (DMOprod) < 54 kg/day, then the <u>EPA/OPPT Small</u> <u>Volume Solids Handling Inhalation Model</u> is used as a default.
- If the daily mass of product output (DMOprod) > 54 kg/day), then either the <u>OSHA Total</u> <u>PNOR PEL-Limiting Model</u> or <u>OSHA Respirable PNOR PEL-Limiting Model</u> may be chosen as a default.

For *batch* operations:

- If the mass of product output per batch (BMOprod) < 54 kg/batch, then the <u>EPA/OPPT</u> <u>Small Volume Solids Handling Inhalation Model</u> is used as a default.
- If the mass of product output per batch (BMOprod) >54 kg/batch, then either the <u>OSHA</u> <u>Total PNOR PEL-Limiting Model</u> or <u>OSHA Respirable PNOR PEL-Limiting Model</u> may be chosen as a default.

NOTE: If the daily amount of material throughput from the Mass Balance calculations was not calculated before the inhalation exposure is calculated, the <u>OSHA Total PNOR PEL-Limiting</u> <u>Model</u> will be used as a default.

EPA Assessment Policy Recommendation: It is recommended that the <u>amount of solid residue</u> that is cleaned from the vessel or process (i.e., the loss fraction x DMOprod or BMOprod) be used to select the default inhalation model, instead using the total capacity of the vessel or process, as described above.

Worker *dermal* exposure to the chemical resulting from this activity is calculated using the <u>EPA/OPPT Direct 2-Hand Dermal Contact with Solids Model</u>

## **Other Release and Exposure Models**

The default release and exposure models assume that the most significant release and exposure during the cleaning operation is from disposal of solid residues containing the chemical and from the generation of dust containing chemical. You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur during cleaning and disposal of solid product residues cleaned from process vessels. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following alternative model may be used to estimate releases that occur from this source. The model may also be selected *in addition* to the default, as appropriate.

User-Defined Loss Rate Model

The following alternative inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- OSHA PEL-Limiting Model for Substance-Specific Particulates
- User-Defined Inhalation Model

The following alternative dermal exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

• EPA/OPPT 2-Hand Dermal Contact with Container Surfaces Model

US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.

User-Defined Dermal Model

# **UNIT OPERATIONS AND PROCESSES**

The following release sources/exposure activities may be selected for operations that include the following processes:

- Aqueous Wash of Organic Mass
- Distillation Column Bottoms Disposal
- Filter Media Changeout
- <u>Grinding and Sanding</u>
- Liquid/Liquid Extraction Solvent Disposal
- <u>Scrubber Releases</u>

### **Aqueous Wash of Organic Mass**

#### Definition

The aqueous wash of organic material containing the chemical, in which the chemical is transferred from the organic material into the aqueous phase. The amount of chemical that is transferred into the aqueous phase is estimated based on its water solubility, by default. This activity uses default models to estimate the release of the chemical and worker exposure to the chemical.

### **Default Releases**

Release of the chemical to *non-air media* with the aqueous phase is calculated using the <u>EPA/OPPT Water Saturation Loss Model</u>.

No default model exists for *releases to air* from this source in ChemSTEER. OPPT assumes that releases to air from this source are insignificant when compared to other sources. If a release to air is expected, you must choose an appropriate model or specify a user-defined release to these media (see *Other Release and Exposure Models*, below).

### **Default Exposures**

Worker *inhalation* exposure to the chemical resulting from this activity is calculated using the <u>User-Defined Inhalation Model</u>.

Worker *dermal* exposure to the chemical resulting from this activity is calculated using the EPA/OPPT 2-Hand Dermal Contact with Liquid Model.

### **Other Release and Exposure Models**

The default release and exposure models assume that the most significant release and exposure during this operation is from the disposal of an aqueous phase containing the chemical. You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur as a result of the aqueous wash of organic material. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following alternative models may be used to estimate releases that occur from this source. These models may also be selected *in addition* to the default, as appropriate.

- <u>EPA/OPPT Penetration Model</u> (for indoor activities; air speed ≤ 100 feet/min)
- <u>EPA/OPPT Mass Transfer Coefficient Model</u> (for outdoor activities; air speed >100 feet/min)
- EPA/OAQPS AP-42 Loading Model
- User-Defined Loss Rate Model
- <u>User-Defined Vapor Generation Rate Model</u>

The following alternative inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- EPA/OPPT Mass Balance Inhalation Model
- OSHA PEL-Limiting Model for Substance-Specific Vapors

There are no alternative dermal exposure models available in ChemSTEER at this time.

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

### **Distillation Column Bottoms Disposal**

#### Definition

The disposal of waste collected from distillation column bottoms that contains the chemical and is estimated to primarily result in the release of the chemical.

### **Default Releases**

Release of the chemical to the environment with the disposal of distillation column bottoms waste is calculated using the <u>User-Defined Loss Rate Model</u>

### **Default Exposures**

No default model exists for worker exposures during this activity in ChemSTEER. OPPT assumes that this activity is closed and automated and that exposures are insignificant when compared to other activities. If exposures are expected, you must choose an appropriate model or specify a user-defined exposure (see *Other Release and Exposure Models*, below).

### **Other Release and Exposure Models**

The default release and exposure models assume that the most significant release during this activity is from the disposal of a distillation column bottoms containing the chemical. You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur as a result of disposing of distillation column bottoms. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following alternative models may be used to estimate releases that occur from this source. These models may also be selected *in addition* to the default, as appropriate.

- EPA/OAQPS AP-42 Loading Model
- User-Defined Vapor Generation Rate Model

The following alternative inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- EPA/OPPT Mass Balance Inhalation Model
- OSHA PEL-Limiting Model for Substance-Specific Vapors
- User-Defined Inhalation Model

The following alternative dermal exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.

User-Defined Dermal Model

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

## Filter Media Changeout

### Definition

The disposal of waste filter media that contains residual amounts of the chemical and that is estimated to result in the release of the chemical and worker exposure to the chemical.

### **Default Releases**

Release of the chemical to the environment with the waste filter media is calculated using the <u>User-Defined Loss Rate Model</u>

#### **Default Exposures**

Worker *dermal* exposure to the chemical resulting from this activity is calculated using the <u>EPA/OPPT Direct 2-Hand Dermal Contact with Solids Model</u>

No default model exists for worker *inhalation exposures* during this activity in ChemSTEER. If dermal exposures are expected, you must choose an appropriate model or specify a user-defined exposure (see *Other Release and Exposure Models*, below).

#### **Other Release and Exposure Models**

The default release and exposure models assume that the most significant release and exposure during this operation is from the disposal of wet filter cake material containing the chemical. You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur as a result of disposing of waste filter media. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following alternative models may be used to estimate releases that occur from this source. These models may also be selected *in addition* to the default, as appropriate.

- <u>EPA/OPPT Penetration Model</u> (for indoor activities; air speed ≤ 100 feet/min)
- <u>EPA/OPPT Mass Transfer Coefficient Model</u> (for outdoor activities; air speed >100 feet/min)
- User-Defined Vapor Generation Rate Model

The following inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- EPA/OPPT Mass Balance Inhalation Model
- OSHA PEL-Limiting Model for Substance-Specific Vapors
- <u>EPA/OPPT Small Volume Solids Handling Inhalation Model</u> (for solid amounts <54 kg per day or per batch)
- <u>OSHA Total PNOR PEL-Limiting Model</u> (for solid amounts >54 kg per day or per batch)
- <u>OSHA Respirable PNOR PEL-Limiting Model</u> (for solid amounts >54 kg per day or per batch)
- OSHA PEL-Limiting Model for Substance-Specific Particulates
- <u>User-Defined Inhalation Model</u>

The following alternative dermal exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- <u>EPA/OPPT 1-Hand Dermal Contact with Liquid Model</u>
- EPA/OPPT 2-Hand Dermal Contact with Liquid Model

<u>US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal</u> <u>Exposure, September 2013.</u>

- EPA/OPPT 2-Hand Dermal Immersion with Liquid Model
- EPA/OPPT 2-Hand Dermal Contact with Container Surfaces Model

<u>US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal</u> <u>Exposure, September 2013.</u>

User-Defined Dermal Model

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

### **Grinding and Sanding**

### Definition

The grinding or sanding of a solid material that contains the chemical and that is estimated to result in the release of the chemical and worker exposure to the chemical.

### **Default Releases**

Release of the chemical to the environment as a result of grinding/sanding activities is calculated using the <u>User-Defined Loss Rate Model</u>.

### **Default Exposures**

This activity is assumed to generate >54 kg of particulates per day, and thus the worker *inhalation* exposure to the chemical resulting from this activity is calculated using either the <u>OSHA Total</u> <u>PNOR PEL-Limiting Model</u>.

Worker *dermal* exposure to the chemical resulting from this activity is calculated using the <u>EPA/OPPT Direct 2-Hand Dermal Contact with Solids Model</u>

### **Other Release and Exposure Models**

The default release and exposure models assume that the most significant release and exposure during this operation is from the generation of dusts containing the chemical. You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur as a result of grinding and/or sanding activities. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

At this time, ChemSTEER does not contain other *release models* that are appropriate for this activity.

The following alternative *inhalation exposure models* may be used to estimate the worker exposure that occurs as a result of performing this activity:

- OSHA Respirable PNOR PEL-Limiting Model
- OSHA PEL-Limiting Model for Substance-Specific Particulates
- User-Defined Inhalation Model

The following alternative *dermal exposure models* may be used to estimate the worker exposure that occurs as a result of performing this activity:

• EPA/OPPT 2-Hand Dermal Contact with Container Surfaces Model

US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.

User-Defined Dermal Model

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

### Liquid/Liquid Extraction Solvent Disposal

### Definition

The disposal of waste solvent containing the chemical that is collected from a liquid-liquid extraction process and is estimated to result in the release of the chemical and worker exposure to the chemical.

### **Default Releases**

Release of the chemical to the environment with the waste solvent is calculated using the <u>User-</u> <u>Defined Loss Rate Model</u>.

### **Default Exposures**

Worker *dermal* exposure to the chemical resulting from this activity is calculated using the <u>EPA/OPPT 2-Hand Dermal Contact with Liquid Model</u>.

No default model exists for worker *inhalation exposures* during this activity in ChemSTEER. You must choose an appropriate model or specify a user-defined exposure (see *Other Release and Exposure Models*, below).

### **Other Release and Exposure Models**

The default release and exposure models assume that the most significant release and exposure during this operation is from the disposal of solvent material containing the chemical. You may have

information and/or data that better represents the chemical releases and/or the worker exposures that occur as a result of disposing of distillation column bottoms. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following alternative models may be used to estimate releases that occur from this source. These models may also be selected *in addition* to the default, as appropriate.

- <u>EPA/OPPT Penetration Model</u> (for indoor activities; air speed ≤ 100 feet/min)
- <u>EPA/OPPT Mass Transfer Coefficient Model</u> (for outdoor activities; air speed >100 feet/min)
- EPA/OAQPS AP-42 Loading Model
- User-Defined Vapor Generation Rate Model

The following inhalation exposure models may be appropriate alternatives for calculating worker exposure that occurs as a result of performing this activity:

- EPA/OPPT Mass Balance Inhalation Model
- OSHA PEL-Limiting Model for Substance-Specific Vapors
- User-Defined Inhalation Model

There are no alternative dermal exposure models available in ChemSTEER at this time.

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

## Scrubber Releases

### Definition

The release of the chemical from a process scrubber device that is also estimated to result in worker exposure to the chemical.

## **Default Releases**

Release of the chemical to the environment from the scrubber device is calculated using the <u>User-Defined Loss Rate Model</u>.

### **Default Exposures**

Worker *inhalation* exposure to the chemical resulting from this activity is calculated using the <u>User-Defined Inhalation Model</u>.

No default model exists for worker *dermal exposures* during this activity in ChemSTEER. If dermal exposures are expected, you must choose an appropriate model or specify a user-defined exposure (see *Other Release and Exposure Models*, below).

### **Other Release and Exposure Models**

The default release and exposure models assume that the most significant release and exposure during this operation is from the release and/or disposal of waste materials containing the chemical from a scrubber device. You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur as a result of the releases from a scrubber device. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following alternative models may be used to estimate releases that occur from this source. These models may also be selected *in addition* to the default, as appropriate.

- <u>EPA/OPPT Penetration Model</u> (for indoor activities; air speed ≤ 100 feet/min)
- <u>EPA/OPPT Mass Transfer Coefficient Model</u> (for outdoor activities; air speed >100 feet/min)
- <u>User-Defined Vapor Generation Rate Model</u>

The following alternative inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- EPA/OPPT Mass Balance Inhalation Model
- OSHA PEL-Limiting Model for Substance-Specific Vapors

There are no alternative dermal exposure models available in ChemSTEER at this time.

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

## VAPOR RELEASE FROM TRANSFER OPERATIONS

The following release source/exposure activity may be selected for operations in which the chemical is volatilized and released from a liquid pool or other type of open liquid surface:

• Vapor Releases from Open Liquid Surfaces

#### Vapor Releases from Open Liquid Surfaces

Definition

The release of chemical vapors as a result of a pool of volatile liquid or other liquid surface that is open to the environment. There may also be a potential for worker inhalation exposures to the chemical vapors.

### **Default Release**

Release of the chemical *to air* is calculated using the <u>User-Defined Vapor Generation Rate Model</u> as a default.

NOTE: the air release model above is only defaulted if the selected operation's adjusted vapor pressure (AVPrm, AVPprod) is within the preferred range of AVPs. Refer to the <u>Operation</u> <u>Parameters Tab  $\rightarrow$  Shared Parameters/Factors Subtab</u> topic for more information. If the operation AVP is outside of the preferred range, there is no model for calculating releases to air from this source.

No default model exists for *releases to non-air media* from this source in ChemSTEER. OPPT assumes that releases from this source are insignificant when compared to other sources. If a release is expected, you must choose an appropriate model or specify a user-defined release to these media (see *Other Release and Exposure Models*, below).

### **Default Exposures**

Worker *inhalation* exposure to the chemical resulting from this activity is calculated using the <u>EPA/OPPT Mass Balance Inhalation Model</u>.

**NOTE**: In order to utilize the above vapor inhalation model, you must select and run a vapor generation release model for this source/activity in order to obtain the necessary input parameters for this model.

**NOTE**: the inhalation exposure model above is only defaulted if the selected operation's adjusted vapor pressure (AVPrm, AVPprod) is within the preferred range of AVPs. Refer to the <u>Operation Parameters Tab  $\rightarrow$  Shared Parameters/Factors Subtab</u> topic for more information. If the operation AVP is outside of the preferred range, there is no model for calculating worker inhalation exposures during this activity.

No default model exists for worker *dermal exposures* during this activity in ChemSTEER. If dermal exposures are expected, you must choose an appropriate model or specify a user-defined exposure (see *Other Release and Exposure Models*, below).

## **Other Release and Exposure Models**

The default release and exposure models assume that the most significant exposure during this operation is from the evaporation of volatile liquid containing chemical vapor from an open surface. You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur during the release of chemical vapor during open transfer operations. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following alternative models may be used to estimate releases that occur from this source. These models may also be selected *in addition* to the default, as appropriate.

- <u>EPA/OPPT Penetration Model</u> (for indoor activities; air speed ≤ 100 feet/min)
- <u>EPA/OPPT Mass Transfer Coefficient Model</u> (for outdoor activities; air speed > 100 feet/min)
- User-Defined Loss Rate Model
- User-Defined Vapor Generation Rate Model

The following alternative inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- OSHA PEL-Limiting Model for Substance-Specific Vapors
- User-Defined Inhalation Model

The following dermal exposure model may be used to estimate the worker exposure that occurs as a result of performing this activity:

US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.

User-Defined Dermal Model

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

## **MISCELLANEOUS SOURCES/ACTIVITIES**

The following may be selected for operations that include either sources of release or worker activities resulting in exposures that you wish to define:

- Miscellaneous Sources/Activities Related to Liquid Processing
- Miscellaneous Sources/Activities Related to Solid Processing

### Miscellaneous Sources/Activities Related to Liquid Processing

#### Definition

A source of release and/or a worker activity involving a liquid containing the chemical that results in the release of the chemical and/or worker exposure to the chemical. This source/activity may be used in the absence of a more suitable choice in ChemSTEER.

### **Default Release**

No default model exists for releases to the environment from this source in ChemSTEER. If a release is expected, you must choose an appropriate model or specify a user-defined release (see *Other Release and Exposure Models*, below).

### **Default Exposures**

Worker *inhalation* exposure to the chemical resulting from this activity is calculated using the User-Defined Inhalation Model.

Worker *dermal* exposure to the chemical resulting from this activity is calculated using the <u>EPA/OPPT 1-Hand Dermal Contact with Liquid Model</u>.

#### **Other Release and Exposure Models**

The default exposure models assume that the most significant exposure during this operation is handling a liquid material containing the chemical. You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur during the activity. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following models may be used to estimate releases that occur from this source. More than one release model may be used at one time to estimate releases, as appropriate.

- <u>EPA/OPPT Penetration Model</u>(for indoor activities; air speed ≤ 100 feet/min)
- <u>EPA/OPPT Mass Transfer Coefficient Model</u> (for outdoor activities; air speed >100 feet/min)
- EPA/OAQPS AP-42 Loading Model
- EPA/OPPT Water Saturation Loss Model
- User-Defined Loss Rate Model
- User-Defined Vapor Generation Rate Model

The following alternative inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- EPA/OPPT Mass Balance Inhalation Model
- OSHA PEL-Limiting Model for Substance-Specific Vapors
- OSHA PEL-Limiting Model for Substance-Specific Particulates
- OSHA Total PNOR PEL-Limiting Model
- OSHA Respirable PNOR PEL-Limiting Model
- EPA/OPPT UV Roll Coating Inhalation Model

The following alternative dermal exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- EPA/OPPT 1-Hand Dermal Contact with Liquid Model
- EPA/OPPT 2-Hand Dermal Contact with Liquid Model

US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.

User-Defined Dermal Model

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

#### Miscellaneous Sources/Activities Related to Solid Processing

#### Definition

A source of release and/or a worker activity involving a solid/particulate containing the chemical that results in the release of the chemical and/or worker exposure to the chemical. This source/activity may be used in the absence of a more suitable choice in ChemSTEER.

#### **Default Release**

No default model exists for releases to the environment from this source in ChemSTEER. If a release is expected, you must choose an appropriate model or specify a user-defined release (see *Other Release and Exposure Models*, below).

#### **Default Exposures**

Worker *inhalation* exposure to the chemical resulting from this activity is calculated using one of the following models:

For continuous operations:

- If the daily mass of product output (DMOprod) < 54 kg/day, then the <u>EPA/OPPT Small</u> <u>Volume Solids Handling Inhalation Model</u> is used as a default.
- If the daily mass of product output (DMOprod) > 54 kg/day), then either the <u>OSHA Total</u> <u>PNOR PEL-Limiting Model</u> or <u>OSHA Respirable PNOR PEL-Limiting Model</u> may be chosen as a default.

For batch operations:

- If the mass of product output per batch (BMOprod) < 54 kg/batch, then the <u>EPA/OPPT</u> <u>Small Volume Solids Handling Inhalation Model</u> is used as a default.
- If the mass of product output per batch (BMOprod) >54 kg/batch, then either the <u>OSHA</u> <u>Total PNOR PEL-Limiting Model</u> or <u>OSHA Respirable PNOR PEL-Limiting Model</u> may be chosen as a default.

NOTE: If the daily amount of material throughput from the Mass Balance calculations was not calculated by ChemSTEER before the inhalation exposure is calculated, the <u>OSHA Total PNOR</u> <u>PEL-Limiting Model</u> will be used as a default.

Worker *dermal* exposure to the chemical resulting from this activity is calculated using the <u>EPA/OPPT Direct 2-Hand Dermal Contact with Solids Model</u>

#### **Other Release and Exposure Models**

The default exposure models assume that the most significant exposure during this operation is handling a solid material containing the chemical. You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur during the activity. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following models may be used to estimate releases that occur from this source. More than one release model may be used at one time to estimate releases, as appropriate.

- EPA/OPPT Water Saturation Loss Model
- User-Defined Loss Rate Model

The following alternative inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- OSHA PEL-Limiting Model for Substance-Specific Particulates
- OSHA PEL-Limiting Model for Substance-Specific Vapors
- EPA/OPPT UV Roll Coating Inhalation Model
- User-Defined Inhalation Model

The following alternative dermal exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

• EPA/OPPT 2-Hand Dermal Contact with Container Surfaces Model

US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.

User-Defined Dermal Model

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

# **AUTOMOBILE SPRAY COATING**

The following release source/exposure activity may be selected for operations in which a liquid coating material containing the chemical is sprayed onto automobile surfaces:

- Automobile OEM Spray Coating Application
- <u>Automobile Refinish Spray Coating Application</u>

### **Automobile OEM Spray Coating Application**

### Definition

The spraying of a liquid coating material onto an automobile surface with a spray gun and within a spray booth with mist capture controls that results in a release of the chemical and/or worker exposure to the chemical.

### **Default Releases**

*Multi-media Release:* The amount of chemical released to both *air and non-air media* as a result of oversprayed mists generated by this activity is calculated using the <u>EPA/OPPT Automobile OEM</u> <u>Coating Overspray Loss Model</u>. This model apportions amounts of the oversprayed mist that is collected by the spraybooth and control technology, as well as the amount of mist that is emitted from the booth to air.

### **Default Exposures**

Worker *inhalation* exposure to the chemical resulting from this activity is calculated using the <u>EPA/OPPT Automobile OEM Spray Coating Inhalation Exposure Model</u>.

Worker *dermal* exposure to the chemical resulting from this activity is calculated using the <u>US</u> <u>EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal</u> <u>Exposure, September 2013.</u> <u>EPA/OPPT 2-Hand Dermal Immersion with Liquid Model.</u>

### **Other Release and Exposure Models**

The default release and exposure models assume that the most significant release and exposure during the automobile spray coating operation is from the generation of coating mists as a result of overspray (or "bounce-back"). You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur during the spray coating of automobiles. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following alternative models may be used to estimate releases that occur from this source. These models may also be selected *in addition* to the default, as appropriate.

- User-Defined Loss Rate Model
- <u>User-Defined Vapor Generation Rate Model</u>
- EPA/OPPT Automobile Refinish Coating Overspray Loss Model

The following alternative inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- OSHA PEL-Limiting Model for Substance-Specific Particulates
- OSHA PEL-Limiting Model for Substance-Specific Vapors

- User-Defined Inhalation Model
- EPA/OPPT Automobile Refinish Spray Coating Inhalation Exposure Model
- <u>EPA/OPPT Automobile Spray Coating Inhalation Exposure Model</u> (non-volatile polyisocyanates)

The following alternative dermal exposure model may be used to estimate the worker exposure that occurs as a result of performing this activity:

US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.

User-Defined Dermal Model

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

#### Automobile Refinish Spray Coating Application

#### Definition

The spraying of a liquid coating material onto an automobile surface with a spray gun and within a spray booth with mist capture controls that results in a release of the chemical and/or worker exposure to the chemical.

#### **Default Releases**

*Multi-media Release:* The amount of chemical released to both *air and non-air media* as a result of oversprayed mists generated by this activity is calculated using the <u>EPA/OPPT Automobile Refinish</u> <u>Coating Overspray Loss Model</u>. This model apportions amounts of the oversprayed mist that is collected by the spraybooth and control technology, as well as the amount of mist that is emitted from the booth to air.

#### **Default Exposures**

Worker *inhalation* exposure to the chemical resulting from this activity is calculated using the <u>EPA/OPPT Automobile Refinish Spray Coating Inhalation Exposure Model</u>.

Worker *dermal* exposure to the chemical resulting from this activity is calculated using the <u>US</u> <u>EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal</u> <u>Exposure, September 2013.</u> EPA/OPPT 2-Hand Dermal Immersion with Liquid Model.

#### **Other Release and Exposure Models**

The default release and exposure models assume that the most significant release and exposure during the automobile spray coating operation is from the generation of coating mists as a result of overspray (or "bounce-back"). You may have information and/or data that better represents the

chemical releases and/or the worker exposures that occur during the spray coating of automobiles. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following alternative models may be used to estimate releases that occur from this source. These models may also be selected *in addition* to the default, as appropriate.

- User-Defined Loss Rate Model
- <u>User-Defined Vapor Generation Rate Model</u>
- EPA/OPPT Automobile OEM Coating Overspray Loss Model

The following alternative inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- OSHA PEL-Limiting Model for Substance-Specific Particulates
- OSHA PEL-Limiting Model for Substance-Specific Vapors
- User-Defined Inhalation Model
- EPA/OPPT Automobile OEM Spray Coating Inhalation Exposure Model
- <u>EPA/OPPT Automobile Spray Coating Inhalation Exposure Model</u> (non-volatile polyisocyanates)

The following alternative dermal exposure model may be used to estimate the worker exposure that occurs as a result of performing this activity:

<u>US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal</u> <u>Exposure, September 2013.</u>

User-Defined Dermal Model

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

# **GENERIC COATING APPLICATIONS**

The following release sources/exposure activities may be selected for operations in which a liquid coating material containing the chemical is applied to a substrate surface:

- Roll Coating
- <u>Coating Using Hand Held Spray Gun</u>
- <u>Coating Using Hand Held Spray Can</u>

## **Roll Coating**

### Definition

The application of a liquid coating material onto a surface or substrate via machine or hand rolling technique that results in a release of the chemical and/or worker exposure to the chemical.

### **Default Releases**

Release of the chemical to the environment from roll coating activity is calculated using the <u>User-Defined Loss Rate Model</u>.

### **Default Exposures**

Worker *inhalation* exposure to the chemical resulting from this activity is calculated using the <u>EPA/OPPT UV Roll Coating Inhalation Model</u>.

No default model exists for worker *dermal exposures* during this activity in ChemSTEER. If dermal exposures are expected, you must choose an appropriate model or specify a user-defined exposure (see *Other Release and Exposure Models*, below).

### **Other Release and Exposure Models**

The default release and exposure models assume that the most significant release and exposure during the roll coating operation is from the generation of coating mists from the moving roller(s). You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur during the spray coating of automobiles. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following alternative models may be used to estimate releases that occur from this source. These models may also be selected *in addition* to the default, as appropriate.

- <u>EPA/OPPT Penetration Model</u> (for indoor activities; air speed ≤ 100 feet/min)
- <u>EPA/OPPT Mass Transfer Coefficient Model</u> (for outdoor activities; air speed >100 feet/min)
- <u>User-Defined Vapor Generation Rate Model</u>

The following alternative inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- EPA/OPPT Mass Balance Inhalation Model
- OSHA PEL-Limiting Model for Substance-Specific Particulates
- OSHA PEL-Limiting Model for Substance-Specific Vapors
- OSHA Total PNOR PEL-Limiting Model
- OSHA Respirable PNOR PEL-Limiting Model
- User-Defined Inhalation Model

The following dermal exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

### • EPA/OPPT 2-Hand Dermal Contact with Liquid Model

<u>US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal</u> <u>Exposure, September 2013.</u>

• User-Defined Dermal Model

**Note to the user:** ChemSTEER currently allows you to select ANY release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity. Please refer to this topic when choosing an appropriate alternative release/exposure model.

### **Coating Using Hand Held Spray Gun**

### Definition

The manual spraying of a liquid coating material onto a surface using a spray gun that results in a release of the chemical and/or worker exposure to the chemical.

### **Default Releases**

No default model exists for releases to the environment from this source in ChemSTEER. If a release is expected, you must choose an appropriate model or specify a user-defined release (see *Other Release and Exposure Models*, below).

### **Default Exposures**

Worker *inhalation* exposure to the chemical resulting from this activity is calculated using the <u>OSHA Total PNOR PEL-Limiting Model</u>.

No default model exists for worker *dermal exposures* during this activity in ChemSTEER. If dermal exposures are expected, you must choose an appropriate model or specify a user-defined exposure (see *Other Release and Exposure Models*, below).

### **Other Release and Exposure Models**

The default exposure model assumes that the most significant exposure during manual spraying is from inhalation of the oversprayed mists. You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur during the spray coating activity. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following models may be used to estimate releases that occur from this source. More than one release model may be used at one time to estimate releases, as appropriate.

- EPA/OPPT Automobile Refinish Coating Overspray Loss Model
- User-Defined Loss Rate Model

• User-Defined Vapor Generation Rate Model

The following alternative inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- OSHA PEL-Limiting Model for Substance-Specific Particulates
- OSHA PEL-Limiting Model for Substance-Specific Vapors
- User-Defined Inhalation Model

The following dermal exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.

• EPA/OPPT 2-Hand Dermal Immersion with Liquid Model

<u>US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal</u> <u>Exposure, September 2013.</u>

User-Defined Dermal Model

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

### **Coating Using Hand Held Spray Can**

### Definition

The manual spraying of a liquid coating material onto a surface using a spray can that results in a release of the chemical and/or worker exposure to the chemical.

### **Default Releases**

No default model exists for releases to the environment from this source in ChemSTEER. If a release is expected, you must choose an appropriate model or specify a user-defined release (see *Other Release and Exposure Models*, below).

### **Default Exposures**

Worker *inhalation* exposure to the chemical resulting from this activity is calculated using the <u>User-Defined Inhalation Model</u>.

No default model exists for worker *dermal exposures* during this activity in ChemSTEER. If dermal exposures are expected, you must choose an appropriate model or specify a user-defined exposure (see *Other Release and Exposure Models*, below).

## Other Release and Exposure Models

The default exposure model assumes that the most significant exposure during manual spraying is from inhalation of the oversprayed mists. You may have information and/or data that better represents the chemical releases and/or the worker exposures that occur during the spray coating activity. You may select alternative models to the default models described above to estimate chemical releases and worker exposures.

The following models may be used to estimate releases that occur from this source. More than one release model may be used at one time to estimate releases, as appropriate.

- EPA/OPPT Automobile Refinish Coating Overspray Loss Model
- User-Defined Loss Rate Model
- <u>User-Defined Vapor Generation Rate Model</u>

The following alternative inhalation exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

- OSHA Total PNOR PEL-Limiting Model
- OSHA PEL-Limiting Model for Substance-Specific Particulates
- OSHA PEL-Limiting Model for Substance-Specific Vapors
- User-Defined Inhalation Model

The following dermal exposure models may be used to estimate the worker exposure that occurs as a result of performing this activity:

<u>US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal</u> <u>Exposure, September 2013.</u>

EPA/OPPT 2-Hand Dermal Immersion with Liquid Model

<u>US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal</u> <u>Exposure, September 2013.</u>

User-Defined Dermal Model

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

# **ELECTROPLATING BATH ADDITIVES**

The following release sources/activities may be selected for operations in which an additive is used within an electroplating bath/solution:

• Operating the Electroplating Bath

- <u>Rinsing Electroplated Parts</u>
- <u>Changing Electroplating Bath</u>

### **Operating the Electroplating Bath**

#### Definition

The use of an additive (containing the chemical being assessed) in electroplating baths/solutions that results in a dermal exposure to the workers who operate the bath (releases of the chemical are not expected during the electroplating process).

### **Default Releases**

No default model exists for releases to the environment from this source in ChemSTEER. If a release is expected, you must choose an appropriate model or specify a user-defined release.

### **Default Exposures**

Worker *inhalation* exposure to the chemical resulting from this activity is calculated using the <u>OSHA PEL-Limiting Model for Substance-Specific Particulates</u>. In this activity, the model uses the **OSHA PEL for chromium (KCk = 0.5 mg/m3)** and an **estimated chromium concentration in an electroplating bath (Ypel=0.25)** as overriding defaults to this model's standard default values.

No default model exists for worker *dermal* exposures during this activity in ChemSTEER. If a dermal exposure is expected, you must choose an appropriate model or specify a user-defined exposure.

## **Other Release and Exposure Models**

You may have information and/or data that support the potential for an environmental release of the chemical during the electroplating process. You may select models to estimate the release. You are encouraged to review the calculations and bases of ChemSTEER's release models (see <u>Quick</u> <u>Summary of ChemSTEER Release Models</u>) prior to using within this source/activity.

You may also have information and/or data that support the potential for worker dermal exposures (or alternative inhalation exposures) during the electroplating process. You may select models to estimate worker inhalation and/or dermal exposures. You are encouraged to review the calculations and bases of ChemSTEER's exposure models (see <u>General Guidelines for Exposure</u> <u>Assessment</u>) prior to using within this source/activity.

Important Note: this source/activity was designed for use within the <u>Electroplating Bath</u> <u>Additive Use</u> operation to use the above described default model. It is recommended that you do NOT alter the default release model selections for this source/activity. If you wish to calculate additional releases from this operation (e.g., empty container residues), you should select the appropriate sources/activities and their associated release/exposure models <u>in</u> <u>addition to</u> the *Operating the Electroplating Bath* activity and the other default sources for this operation. You are encouraged to review the bases and default models used by the other sources/activities (see <u>Operations Tab  $\rightarrow$  Sources/Activities Subtab</u>) prior to selecting other sources/activities for this operation. The *Changing Electroplating Bath* source/activity can NOT be used within any other operation than the *Electroplating Bath Additive Use* operation.

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

### **Rinsing Electroplated Parts**

#### Definition

The use of an additive (containing the chemical being assessed) in electroplating baths/solutions that results in a release of the chemical (worker exposures are not expected after the chemical is added to the bath).

### **Default Releases**

*Multi-media Release:* The amount of chemical released to both *water* and *land or incineration* as a result of rinsing the chemical from electroplated parts surfaces is calculated using the EPA/OPPT Electroplating Rinse Water Loss Model. This model apportions amounts of chemical in the rinsate that are removed from the process wastewater by the treatment system and disposed with the sludge, as well as the amount of chemical that is discharged to water with the final effluent.

### **Default Exposures**

No default model exists for worker exposures during this activity in ChemSTEER. OPPT assumes that workers do not come into contact with the additive while it is rinsed from electroplated parts. If exposures are expected, you must choose an appropriate model or specify a user-defined exposure.

### **Other Release and Exposure Models**

You may have information and/or data that support the potential for worker exposures during the rinsing of the electroplated part. You may select models to estimate worker exposures. You are encouraged to review the calculations and bases of ChemSTEER's exposure models (see <u>General</u> <u>Guidelines for Release Assessment</u>) prior to using within this source/activity.

Important Note: this source/activity was designed for use within the <u>Electroplating Bath</u> <u>Additive Use</u> operation to use the above described default model. It is recommended that you do NOT alter the default release model selections for this source/activity. If you wish to calculate additional releases from this operation (e.g., empty container residues), you should select the appropriate sources/activities and their associated release/exposure models <u>in</u> <u>addition to</u> the *Rinsing Electroplated Parts* source and the other default sources/activities for this operation. You are encouraged to review the bases and default models used by the other sources/activities (see <u>Operations Tab  $\rightarrow$  Sources/Activities Subtab</u>) prior to selecting other sources/activities for this operation. The *Rinsing Electroplated Parts* source/activity can NOT be used within any other operation than the *Electroplating Bath Additive Use* operation.

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

### **Changing Electroplating Bath**

#### Definition

The use of an additive (containing the chemical being assessed) in electroplating baths/solutions that results in a release of the chemical (worker exposures are not expected after the chemical is added to the bath).

#### **Default Releases**

*Multi-media Release:* The amount of chemical released to both water and land or incineration as a result of changing the electroplating bath solution is calculated using the EPA/OPPT Electroplating Spent Bath Disposal Model. This model apportions amounts of chemical in the spent bath that are removed by the treatment system and disposed with the sludge, as well as the amount of chemical that is discharged to water with the final effluent.

#### **Default Exposures**

No default model exists for worker exposures during this activity in ChemSTEER. OPPT assumes that workers do not come into contact with the additive during the spent bath wastewater treatment or discharge. If exposures are expected, you must choose an appropriate model or specify a user-defined exposure.

### **Other Release and Exposure Models**

You may have information and/or data that support the potential for worker exposures during the treatment and discharge of the electroplating additive. You may select models to estimate worker exposures. You are encouraged to review the calculations and bases of ChemSTEER's exposure models (see <u>General Guidelines for Exposure Assessment</u>) prior to using within this source/activity.

Important Note: this source/activity was designed for use within the Electroplating Bath Additive Use operation to use the above described default model. It is recommended that you do NOT alter the default release model selections for this source/activity. If you wish to calculate additional releases from this operation (e.g., empty container residues), you should select the appropriate sources/activities and their associated release/exposure models in addition to the Rinsing Electroplated Parts source and the other default sources/activities for this operation. You are encouraged to review the bases and default models used by the other sources/activities (see Operations Tab  $\rightarrow$  Sources/Activities Subtab) prior to selecting other sources/activities for this operation. The *Changing Electroplating Bath* source/activity can NOT be used within any other operation than the *Electroplating Bath Additive Use* operation.

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

## **RECIRCULATING WATER-COOLING TOWER ADDITIVES**

The following release source may be selected for operations in which an additive is used within recirculating water-cooling towers:

• <u>Recirculating Water-Cooling Tower Additive Releases</u>

### **Recirculating Water-Cooling Tower Additive Releases**

#### Definition

The use of an additive (containing the chemical being assessed) to recirculating water-cooling tower systems that results in a release of the chemical (worker exposures are not expected after the chemical is added to the system).

#### **Default Releases**

Air Release:

Release of the chemical contained in the additive as a result of windage losses of the recirculating fluid (e.g., water) mists is calculated using the <u>EPA/OPPT Cooling Tower Windage Loss</u> <u>Model</u>.

Release of the chemical (if volatile) as a result of the evaporation of the recirculating fluid is calculated using the <u>EPA/OPPT Cooling Tower Evaporative Loss Model (volatiles)</u>.

**NOTE**: the air release model above is only defaulted if the selected operation's adjusted vapor pressure (AVPrm, AVPprod) is within the preferred range of AVPs. Refer to the <u>Operation</u> <u>Parameters Tab  $\rightarrow$  Shared Parameters/Factors Subtab</u> topic for more information. If the operation AVP is outside of the preferred range, there is no model for calculating releases to air from this source.

### Water Release:

Release of the chemical contained in the additive as a result of the periodic blowdown of the recirculating fluid is calculated using the <u>EPA/OPPT Cooling Tower Blowdown Loss Model</u>.

### **Default Exposures**

No default model exists for worker exposures during this activity in ChemSTEER. OPPT assumes that once the additive enters the recirculating water-cooling tower system, workers do not come into contact with the additive during its use or release. If exposures are expected, you must choose an appropriate model or specify a user-defined exposure.
# **Other Release and Exposure Models**

You may have information and/or data that support the potential for worker exposures during the use of the water-cooling tower additive. You may select models to estimate worker exposures. You are encouraged to review the calculations and bases of ChemSTEER's exposure models (see <u>General</u> <u>Guidelines for Exposure Assessment</u>) prior to using within this source/activity.

Important Note: this source/activity was designed for use within the <u>Recirculating Water-Cooling Tower Additive Use</u> Operation to use the above described default models. It is recommended that you do NOT alter the default release model selections for this source/activity. If you wish to calculate additional releases from this operation (e.g., empty container residues), you should select the appropriate sources/activities and their associated release/exposure models in addition to the *Recirculating Water-Cooling Tower Additive Releases* source. You are encouraged to review the bases and default models used by the other sources/activities (see <u>Operations Tab  $\rightarrow$  Sources/Activities Subtab</u>) prior to selecting other sources/activities for this operation.

The *Recirculating Water-Cooling Tower Additive Releases* source/activity can NOT be used within any other operation than the *Recirculating Water-Cooling Tower Additive Use* operation.

**Note to the user:** ChemSTEER currently allows you to select *ANY* release or exposure model contained in the software to calculate release amounts and worker exposures. Be aware that not all of the models contained in the software are appropriate for a particular source/activity.

Please refer to this topic when choosing an appropriate alternative release/exposure model.

# **ChemSTEER Estimation Methods and Models**

The environmental release models are accessed on the <u>Estimating Chemical Releases Tab</u> and the inhalation and dermal exposure models are accessed on the <u>Estimating Chemical Exposures Tab</u>.

You must have selected at least one operation with at least one source/activity (see <u>Operations</u> <u>Tab  $\rightarrow$  Sources/Activities Subtab</u> section) in your assessment in order to run any of the release or exposure models. You are also required to provide any input parameter values that are required by the model and for which ChemSTEER does not have a default value.

Complete documentation for each of the environmental release and worker exposure models is located in pages of this User Guide section. Each of the model topics describes type of release or exposure that the model calculates, default target environmental media or route of exposure, and the form of the chemical. Definitions, all equations and input parameters, descriptions of all default values and associated logic behind conditional defaults, as well as any non-default options for each of the input parameters are also provided.

The methods and models used in ChemSTEER are from several EPA sources, including the "Chemical Engineering Branch Manual for the Preparation of Engineering Assessments" and other reports and memoranda detailing the methods used in CEB assessments. References to the industryspecific operations are taken from the "Chemical Engineering Branch Compilation of Generic Scenarios for Chemical Uses." These references document the various empirical, mathematical, and suppositional methods and models that have been developed and used by EPA over many years of workplace exposure and release assessment.

To review a complete list of references used in ChemSTEER, go to the <u>References</u> section of this User Guide.

The environmental release model topics are organized by target environmental media (air, nonair, and multi-media), as well as by the form of the chemical when released (vapor, liquid, solid) and associated mechanism of release (evaporation, residual and waste).

The worker exposure model topics are organized by route of exposure (inhalation and dermal), form of the chemical during the activity (liquid, solid) and mechanism (evaporation, vapor displacement, misting, dusting, and dermal contact with the chemical or surfaces). There is also a section that contains the set of exposure models based on exposure limits.

# **GENERAL INFORMATION ON MODEL PARAMETERS**

# **Changing Default Values**

You may elect to change any model parameter to an alternative value to the default. To do this, click on the Type column for the parameter. For most parameters you have two choices:

- ChemSTEER defaults for that model; and
- User-defined.

Some model parameters have more than these two options for designating input values. In addition, some model parameters (i.e., those that are generated by another model) cannot be changed. These parameters are designated with 'Model Output' in the *Type* column.

Be sure to read the specific model documentation topic in this User Guide for a complete description of each parameter's non-default options.

# Note About Frequency of Release (Freq) Values

If you select a non-default Freq or enter a User-defined Freq with a value greater than 365, ChemSTEER will display a pop-up message warning you that the choice is invalid because it exceeds 365 days/yr. You must then choose an option that will result in Freq < 365 days/yr before ChemSTEER will allow you move on from the selection process.

# Note About Exposure Days per Year (ED) Values

If you select a non-default ED or enter a User-defined ED with a value greater than 365, ChemSTEER will display a pop-up message warning you that the choice is invalid because it exceeds 365 days/yr. You must then choose an option that will result in ED < 365 days/yr before ChemSTEER will allow you move on from the selection process.

# The Parameter Type Column

ChemSTEER will indicate whether the parameter used is the ChemSTEER default or a userselected non-default parameter in the *Parameter Type* Column.

# The Value Calc Column

In the *Value Calc* column, ChemSTEER displays the equation or parameter origin (tab location) that was used to generate the value used in the model equation.

# **Running the Model**

After you have updated the model parameters and click the *Run Model* button, ChemSTEER updates all of the model results for the selected operation. If the total annual release (AR) is greater than the operation's total production volume (PVop), ChemSTEER will display a pop-up message warning you that the annual release for this model exceeds the volume estimated for this operation; however ChemSTEER will allow you to continue.

# CALCULATING TWO SETS OF RESULTS FROM A SINGLE MODEL

This function is designed to allow you to perform concurrent calculations of two model results from two sets of input parameters. These sets of input parameters and outputs are generally labeled *Output 1* and *Output 2*; however, you can characterize the results by selecting from a pick-list of choices or by entering a short description of your own. For example, this feature can be used to calculate <u>a</u> range of model results using a range in at least one input parameter value.

# Model Input Parameter Columns and On/Off Switches

Each model input parameter has a *Units, Type, Origin,* and *Value* column.

For the <u>release model input parameters</u>, these are displayed in both the Releases tab - *Release Input Parameters* subtab and the *View/Update Release Model Information* screen.

Likewise, for the <u>exposure model input parameters</u>, these are displayed on the *Exposures* tab - (*Dermal* or *Inhalation*) *Model Input Parameters* subtabs and the *View/Update Exposure Model Information* screen.

In the View/Update (Release or Exposure) Model Information screens, there are two check boxes (Enable Model Parameters for Output 1 and Enable Model Parameters for Output 2) that allow you to turn on/off each of two sets of parameter values. By checking each of the boxes, the associated set of parameter columns will be displayed in the View/Update (Release or Exposure) Model Information screens; the Releases tab - Release Input Parameters subtab; and the Exposures tab - (Dermal or Inhalation) Model Input Parameters subtabs. When both boxes are checked, both sets of parameter values will be used by the selected release or exposure model (as applicable) and will cause two results to be calculated by the model.

Each set of input parameters will be displayed in the appropriate columns. For example, input parameters for Output 1 will appear in columns labeled *Type - Output 1*, *Origin - Output 1*, and *Value - Output 1*. Likewise, the input parameters for Output 2 will appear in columns labeled *Type - Output 2*, *Origin - Output 2*, and *Value - Output 2*.

NOTE: each of the release models selected in the assessment will have a separate Output 1/Output 2 setting. In other words, some models will be run for one output as a default, while others are run for both outputs. Each of the User Guide topics for the release/exposure models describe the particular input parameter default values for *Output 1* and/or *Output 2*. These topics also state which of the sets of parameters is enabled <u>by default</u>. Where there is only one default value for an input parameter, the default will be the same for *Output 1* and *Output 2*.

You may enable/disable either one of the model parameter sets by toggling the check boxes. If you disable one of the sets of parameter values, those values will not be displayed on the *Releases or Exposures* tab screens, as appropriate; however, ChemSTEER will retain that set of input parameter values such that if the box is enabled again in the assessment, the set of values can be recalled.

For example, you can enable both boxes, enter several *Output 2* parameter values, run the model, and print a report showing both model output values. Later, you want to generate a report of a more conservative (i.e., higher) model output values, designated as *Output 1*. You would disable the *Output 2* parameter values, run the model and subsequently, the report. Again, at a future time, you wish to call up the assessment again to use as a basis for a similar new assessment. You will be able to re-enable the *Output 2* values to view them and/or reprint the report.

You may also disable both outputs, for example if you wish to temporarily exclude a release source from an operation's combined releases.

#### **Default Parameter Values**

As a general default, both *Output 1* and *Output 2* values for a single parameter are equivalent (unless a particular model contains two accepted default values). If you enable the *Output 2* parameters (by clicking on the check box), you may enter a new value (if the parameter allows for user-specified values) or select from the set of appropriate non-default options; however, ChemSTEER will allow any and all input parameters for *Output 1* and *Output 2* to be equivalent.

Some model parameter values are based on inputs entered on other tabs (e.g., MW from the *Chemical* tab; and NS from the *Mass Balance Parameters* subtab of the *Operation Parameters* tab). These parameter values will default to the value entered in the other ChemSTEER screens, as described in each model's User Guide topic, regardless of which of the *Output 1/Output 2* parameter sets are enabled. If both of the *Enable Model Parameters for Output 1/Output 2* boxes are checked, both of the parameter values will be equivalent by default. For example, the chemical's molecular weight (MW) from the *Chemical* tab will be used as the default for both the *Output 1* and the *Output 2* in the *Releases or Exposures* tab in this case. You may then elect to change one or both parameter values at the model level, preserving the value entered in the originating ChemSTEER screen.

In cases where an exposure model obtains default values from those used or generated by an associated release model, the input parameters for the exposure model *Output 1* will be obtained from those values used for the associated release model *Output 1*; and the input parameters for the exposure model *Output 2* will be obtained from those values used for the associated release model *Output 2*. If you ran the associated release model with either *Output 1* or *Output 2* disabled, some of the model-generated parameters may not be available for the associated exposure model inputs. For example, if you run the *AP-42 Loading Model* only for *Output 1* (i.e., *Output 2* is disabled) and then attempt to run the *Mass Balance Inhalation Model* for both *Output 1* and *Output 2*, the value for G for *Output 2* will be zero.

When ChemSTEER finds that an input parameter has not been specified or calculated, a message is displayed that specifies which input parameter needs to be calculated or entered in order to run the release or exposure model. This message also specifies for which output (i.e., *Output 1* or *Output 2*) the input parameter is required.

# Model Result Characterization Selection/Entry

There are two combo boxes located in the *View/Update (Release and Exposure) Model Information* screens: *Characterization of Output 1 Results*, and *Characterization of Output 2 Results*. These allow you to characterize the model results by either selecting a descriptor from a list, or entering your own characterization descriptor. These labels can also be used to further document the ChemSTEER release and exposure model results within the software.

In a future version of ChemSTEER, when you will have the ability to customize your release and exposure combinations, these individual model result characterizations may be exported into the IRER or other future ChemSTEER reports.

The following is the list of characterization descriptors for each of these combo boxes:

- Output 1 (default for *Output 1*, unless otherwise defaulted by the model)
- Low End of Range

- Average
- Median
- Central Tendency
- Typical
- High End of Range
- High End
- Conservative
- Bounding
- Maximum Based on Limit of Detection
- Worst Case
- What-If
- User-Input (if this option is selected, the combo box will allow the user to key in their own descriptor (up to 25 characters)).

NOTE: for some release and exposure models, an alternative default characterization descriptor may be specified based on the characterization of the default model input parameter values. Please refer to the individual model User Guide topic descriptions for any overriding defaults to the generic setting described above.

The current settings for each of these characterizations is displayed with the model results in the *Estimated Releases* and *Activity Exposure Estimates* subtabs

It is important for you to be consistent in how you enter the alternate input values for *Output 1* and *Output 2* and to be aware that the characterizations chosen or entered (as described above) are for the model <u>results</u>. The *Output 1* parameters provide for the <u>Output 1 model **result**</u> and the *Output 2* parameters provide for the <u>Output 2 model **result**</u>. For example, if you wish to calculate a range in model results based on a range in input data, you could characterize *Output 1* results as "Low End of Range" and *Output 2* results as "High End of Range". What is important to note is that the *Output 1* input parameter values will not necessarily be less than the *Output 2* parameter values. In other words, if the parameter is <u>inversely</u> related to the model result (e.g., it is a denominator in the equation), the *Output 1 = Low End of Range* model parameter value will be greater than the *Output 2 = High End of Range* model parameter value will be greater than the *Output 2 = High End of Range* model parameter value will be greater than the *Output 2 = High End of Range* model parameter value will be greater than the *Output 2 = High End of Range* model parameter value will be greater than the *Output 2 = High End of Range* model parameter value will be greater than the *Output 2 = High End of Range* model parameter value will be greater than the *Output 2 = High End of Range* model parameter value will be greater than the lower the calculation result value).

# **Release Model Results**

Each calculated release result is displayed in the following seven columns on the *Releases* tab - *Estimated Releases* subtab:

- Media;
- Characterization of Results;
- Number of Sites;

- Days of Release;
- Daily Release Rate;
- Annual Release Rate; and
- Basis.

The *Characterization of Results* column contains the characterization settings for each of the output sets (i.e., Output 1 and Output 2) for each receiving environmental medium.

Based on the enable/disable status of the *Enable Model Parameters for Output 1* and *Enable Model Parameters for Output 2* boxes in the *View/Update Release Model Information* screen when the *Run Model(s)* button is clicked, the appropriate set(s) of release results are displayed in the *Estimated Releases* subtab in <u>one or two rows</u> for each media of release.

The values displayed in the columns are derived by running the model calculation. When the *Run Model(s)* button is clicked, the model will perform two calculations (i.e., one for Output 1 and one for Output 2) regardless of which of the outputs is enabled; however, ChemSTEER will only <u>display</u> the appropriate output result(s) in the *Estimated Releases* subtab, as described above. The *Output 1* model parameters will be used as a set to calculate the *Output 1* result values, and the *Output 2* model parameters will be used as a set to calculate the *Output 2* result values.

# **Exposure Model Results**

Each calculated exposure result is displayed in the following nine columns on the *Exposures* tab - *Activity Exposure Estimates* subtab:

- Route of Exposure;
- Characterization of Results;
- Total Number of Workers;
- Exposure Days per Year;
- Estimate Potential Dose Rate (mg/worker-day);
- Lifetime Average Daily Dose (mg/kg-day);
- Average Daily Dose (mg/kg-day);
- Acute Potential Dose (mg/kg-day); and
- Basis.

The *Characterization of Results* column contains the characterization settings for each of the output sets (i.e., *Output 1* and *Output 2*) for each route of exposure.

Based on the enable/disable status of the *Enable Model Parameters for Output 1* and *Enable Model Parameters for Output 2* boxes in the *View/Update Exposure Model Information* screen when the *Run Model(s)* button is clicked, the appropriate exposure results are displayed in the *Activity Exposure Estimates* subtab in <u>one or two rows</u> for each route of exposure.

The values displayed in the columns are derived by running the model calculation. When the *Run Model(s)* button is clicked, the model will perform two calculations (i.e., one for Output 1 and one for Output 2) regardless of which of the outputs is enabled; however, ChemSTEER will only <u>display</u> the appropriate output result(s) in the *Activity Exposure Estimates* subtab, as described above. The Output 1 model parameters will be used as a set to calculate the Output 1 result values, and the Output 2 model parameters will be used as a set to calculate the Output 2 result values.

# Passing Vapor Generation Parameters from the Air Release Model to the Inhalation Exposure Model

When the release of a volatile chemical is assessed in ChemSTEER, the release model calculates a vapor generation rate (G). This parameter is then used to calculate the daily release of the chemical to air. To read more about these types of release models, go to the <u>Models for Calculating Releases to Air</u> section of this User Guide.

The G parameter, as well as other model input parameters (e.g., hours per day, the vapor pressure correction factor (X), and the chemical's vapor pressure), that are calculated or set in the selected release model are then passed to and used by the <u>EPA/OPPT Mass Balance Inhalation Model</u> to calculate the corresponding worker exposure to the chemical vapor on the Exposures tab.

In general, the Output 1 release model parameters will be passed to the Output 1 exposure model parameters and the Output 2 release model parameters will be passed to the Output 2 exposure model parameters. Because ChemSTEER only calculates model outputs, such as G, for enabled outputs, ChemSTEER may substitute values from a non-corresponding output if only one release output is enabled. In order to insure transfer of linked values from release models to exposure models, you should always re-run the release models after updating release values and re-run the exposure models to incorporate these new values in the exposure results.

**Example 1:** You choose to run a vapor generation air release model (e.g., the EPA/OAQPS AP-42 Loading Model) in the Releases tab for Output 2 only. You also modify the hours per day (OHa) of the release from a default of 4 hours per day to 1 hour per day and run or re-run the models.

You then wish to calculate a range of inhalation exposure values using the EPA/OPPT Mass Balance Inhalation Model by enabling both the Output 1 and Output 2 results. The inhalation model hours per day (h) for Output 2 will default to the user-specified OHa for the release (1 hour per day). In addition, Output 1 for the exposure model will be set to the only enabled release model OHa value of 1 hour per day.

If you wish to modify the exposure model Output 1 duration, you may enter user-specified values for the desired parameters in the *View/Update Inhalation Model Information* window, <u>provided they are independently used by the inhalation model equations</u>. If you wish to modify a parameter that is passed from the air release model (e.g., G, duration, etc.), it is recommended that you <u>return to the Releases tab</u>, click on the *View/Update Model Information* button, enable Output 1 parameters, enter the desired Output 1 duration (OHa), and re-run the air release model to re-calculate the G value for Output 1. By changing the duration in the release model, ChemSTEER will calculate the appropriate G value for that duration and pass both values to the inhalation exposure model. ChemSTEER will not prohibit you from changing the duration for Output 1 in the exposure model; however, it will not correspond with the G value that was calculated using the release model defaults.

*Example 2:* You choose to run a vapor generation air release model for Output 2 only, as described in Example 1 above.

You then wish to calculate a <u>single</u> inhalation exposure value for Output 1 only (i.e., Output 2 parameters are disabled). In this case, the exposure model Output 1 parameters will default to the appropriate release model Output 2 values (e.g., vapor generation rate (G) and the duration hours per day). If you later enable the exposure model Output 2 parameters, they will initially default to the exposure model Output 2 values, as specified in the model User Guide topic, and any linked values from the release model Output 2 parameters. If you wish to calculate two results for the exposure model, you may enter user-specified values for the desired parameters in the *View/Update Inhalation Model Information* window, provided they are independently used by the inhalation model equations. If you wish to modify a parameter that is passed from the air release model (e.g., G, duration, etc.) you must follow the instructions described for Example 1.

# **Dual Outputs in the IRER**

If the IRER report is generated while either or both of the *Enable Model Parameters for Output 1* and *Enable Model Parameters for Output 2* boxes are checked, it will include one or both sets of the calculated results, as appropriate.

The "Release Total" (appearing in the IRER only) is calculated by adding together all releases from all sites over all days. Within a release, ChemSTEER will use the greater value from either the Output 1 or Output 2 result for the Release Total.

To read more about the IRER report, go to the <u>IRER Format Details</u> topic.

# **ENVIRONMENTAL RELEASES**

# General Guidelines for Release Assessment

Detailed descriptions of the environmental release models are contained in several User Guide topics, organized according to the type of release (e.g., liquid or solid) and media of release (e.g., to air or other media). Simply click on the desired grouping of models in the User Guide Table of Contents to access these detailed descriptions.

Each manufacturing, processing, and use operation to be assessed is analyzed to determine the sources/activities that can result in releases to the environment that are to be estimated. Once these sources/activities are identified, a general hierarchy of preference may be used to determine how to quantify each release from each source/ activity. The following list shows the potential methods for quantifying releases in order (generally) from the most preferred to the least preferred:

- 1. Measured release monitoring data for the chemical, including concentration and flow rate monitoring data.
- 2. Measured release monitoring data for a "surrogate" chemical with similar "releaseaffecting" properties and used in the same (or very similar) process.
- 3. Modeled release estimates:

- Simulated release estimates (e.g. process design software or mathematical model) for the chemical.
- Regulated limits as an estimated "upper bound" of release.
- "Rule-of-thumb" release estimates, or those developed using analogous points of reference and engineering judgment.

This order of preference is expected to apply generally to most cases of release assessment. However, judgment may dictate that, in some cases, the order within the hierarchy should be changed. Examples of such a change of hierarchy order may include when data are judged to be unreliable or unrepresentative for a particular reason. Also, some estimates may be a combination of two or more of these methods.

Estimation methods in ChemSTEER are based on a combination of factors:

- Research and knowledge of and data from unit operations and industrial processes,
- Some basic chemical engineering principles, and
- Professional experience and judgment.

The standard methods and models in ChemSTEER have been developed to estimate releases for a variety of industrial and commercial operations.

# Quick Summary of ChemSTEER Release Models

All of the ChemSTEER release models are summarized in the table below. For each model, a brief description of the primary calculation(s), as well as a list of the ChemSTEER release sources (or source categories) that use the model as the default for calculating releases, is provided.

NOTE: This table is intended to provide you a "snapshot" of the various ChemSTEER models to help you become more familiar with them. You are highly encouraged to review the full description of the models (provided in this section of the User Guide), as well as the source/activity topics (provided in the <u>Release Sources and Exposure Activities</u> section of the User Guide), for a more complete description of the calculations and logic used.

Quick Summary of ChemSTEER Release Models				
Release Model	Brief Description of Calculation or Basis of Daily Chemical Release (kg/site-day)	Sources That Use the Model as a Default for Calculating Releases		
<b>Models for Calculating Releases of Chemical Vapor to Air</b> NOTE: These models only appear as default for calculating release of a volatile chemical (i.e., the adjusted vapor pressure (AVP) of the material being h is within the specified AVP range).				
EPA/OAQPS AP-42 Loading Model	Daily Release=G x OHa x (3600 s/hr)/(1000 g/kg) Where: G*=vaporization rate (g/s) (uses model equation for loading activities) OHa=hours per site-day for the activity *Be sure to read this model's User Guide topic for more information on how the vaporization rate is calculated	<u>Loading Liquids</u> into Transport Containers/Vessels (all source types)		
EPA/OPPT Mass Transfer Coefficient Model (Use for OUTDOOR sources of release)	Daily Release=G x OHa x (3600 s/hr)/(1000 g/kg) Where: G*=vaporization rate (g/s) (uses model equation for OUTDOOR sources) OHa=hours per site-day for the activity *Be sure to read this model's User Guide topic for more information on how the vaporization rate is calculated.	Cleaning Liquid Residuals from <u>Tank Trucks</u> Used to Transport Raw Material/Product Cleaning Liquid Residuals from <u>Rail Cars</u> Used to Transport the Raw Material/Product Equipment Cleaning Losses <u>of Liquids</u> (all source types)		
<i>EPA/OPPT Penetration Model</i> (Use for INDOOR sources of release)	Daily release=G x OHa x (3600 s/hr)/(1000 g/kg) Where: G*=vaporization rate (g/s) (uses model equation for INDOOR sources) OHa=hours per site-day for the activity *Be sure to read this model's User Guide tonic for more	Cleaning Liquid Residuals from <u>Bottles</u> Used to Transport the Raw Material/Product Cleaning Liquid Residuals from <u>Small Containers</u> Used to Transport the Raw Material/Product Cleaning Liquid Residuals from <u>Totes</u> Used to Transport the Raw Material/Product		
	information on how the vaporization rate is calculated.	Cleaning Liquid Residuals from Storage/Transport		

		Vessels (user-defined material)
		Sampling <u>Liquids</u> (all source types)
User-Defined Vapor Generation Rate Model	Daily release=G x OHa x (3600 s/hr)/(1000 g/kg)	Vapor Releases from Open Liquid Surfaces
	Where:	NOTE: You may choose this model for any source for
	G=vaporization rate (g/s) (you must enter a value)	which you wish to enter a known value for G.
	OHa=hours per site-day for the activity	
EPA/OPPT Cooling Tower Evaporative Loss Model	Daily release=LF x Amt	Recirculating Water-Cooling Tower Additive Releases
	Where:	NOTE: This model cannot be chosen as an alternative
(Used in the Recirculating Water-	LF=loss fraction; between 0.5 and 3 percent (the loss	for any other ChemSTEER sources.
Cooling Tower Additive Use operation)	fraction must be entered and used in the Mass Balance Parameters subtab calculations)	
	Amt=Daily amount of chemical contained in the recirculating	
	entered/calculated in the Mass Balance Parameters subtab)	
Models for Calculating Releases from Tr	ansport Container Residues to Non-Air Media (i.e., water, incin	eration, and/or landfill)
EPA/OPPT Bulk Transport Residual	Daily release=LF x Amt	Cleaning Liquid Residuals from Totes Used to
Model	Where	Transport the Raw Material/Product
	LF=loss fraction; up to 0.2 percent	Cleaning Liquid Residuals from Tank Trucks Used to
		Transport the Raw Material/Product
	Amt*=amount of chemical (kg/site-day) to which the loss	Cleaning Liquid Residuals from Pail Care Used to
	container)	Transport the Raw Material/Product
	*Be sure to read this model's User Guide topic for more	
	information on how the daily amount of chemical is determined.	
EPA/OPPT Drum Residual Model	Daily Release=LF x Amt	Cleaning Liquid Residuals from Drums Used to
	Where:	Transport the Raw Material/Product
		<u> </u>

	LF=loss fraction; <u>up to 3 percent</u> Amt*=amount of chemical (kg/site-day) to which the loss fraction is applied (e.g., daily amount unloaded from container) *Be sure to read this model's User Guide topic for more information on how the daily amount of chemical is determined.	Cleaning Liquid Residuals from <u>Containers (user- defined)</u> Used to Transport the Raw Material/Product Cleaning Liquid Residuals from Storage/Transport Vessels ( <u>user-defined material</u> )
EPA/OPPT Small Container Residual Model	Daily release=LF x Amt Where: LF=loss fraction; <u>up to 0.6 percent</u> Amt*=amount of chemical (kg/site-day) to which the loss fraction is applied (e.g., daily amount unloaded from container) *Be sure to read this model's User Guide topic for more information on how the daily amount of chemical is determined.	Cleaning Liquid Residuals from <u>Bottles</u> Used to Transport the Raw Material/Product Cleaning Liquid Residuals from <u>Small Containers</u> Used to Transport the Raw Material/Product
EPA/OPPT Solid Residuals in Transport Containers Model	Daily release=LF x Amt Where: LF=loss fraction; <u>1 percent</u> Amt*=amount of chemical (kg/site-day) to which the loss fraction is applied (e.g., daily amount unloaded from container) *Be sure to read this model's User Guide topic for more information on how the daily amount of chemical is determined.	Cleaning <u>Solid Residuals</u> from Transport Containers/Vessels (all source types) Equipment Cleaning Losses of <u>Solids</u>
Models for Calculating Releases from Pr	ocess Equipment Vessel Cleaning Residues to Non-Air Media (i.	e., water, incineration, and/or landfill)
EPA/OPPT Multiple Process Vessel	Daily release=LF x Amt	Equipment Cleaning Losses of Liquids from Multiple

Residual Model	Where: LF=loss fraction; <u>2 percent</u>	Vessels
	Amt*=amount of chemical (kg/site-day) to which the loss fraction is applied (e.g., daily amount unloaded from container)	
	*Be sure to read this model's User Guide topic for more information on how the daily amount of chemical is determined.	
EPA/OPPT Single Process Vessel Residual Model	Daily release=LF x Amt Where:	Equipment Cleaning Losses of Liquids from a <u>Single</u> <u>Vessel</u> (all source types)
	LF=loss fraction; <u>up to 1 percent</u>	
	Amt*=amount of chemical (kg/site-day) to which the loss fraction is applied (e.g., daily amount unloaded from container)	
	*Be sure to read this model's User Guide topic for more information on how the daily amount of chemical is determined.	
EPA/OPPT Solid Residuals in Transport Containers Model	Daily release=LF x Amt	Cleaning <u>Solid Residuals</u> from Transport Containers/Vessels (all source types)
	Where: LF=loss fraction; <u>1 percent</u>	Equipment Cleaning Losses of Solids
	Amt*=amount of chemical (kg/site-day) to which the loss fraction is applied (e.g., daily amount unloaded from container)	
	*Be sure to read this model's User Guide topic for more information on how the daily amount of chemical is determined.	
Models for Calculating Releases from Ind	dustry-Specific Sources	

EPA/OPPT Automobile OEM Coating Overspray Loss Model (non-volatile)	Daily release=LF x Amt	Automobile <u>OEM</u> Spray Coating Application
(used in the Automobile OEM Spray Coating Operation)	LF=loss fraction; 1 – TE <u>TE=transfer efficiency of the spray gun (25-65%)</u>	
	Amt*=amount of chemical (kg/site-day) to which the loss fraction is applied (e.g., daily amount unloaded from container)	
	*Be sure to read this model's User Guide topic for more information on how the daily amount of chemical is determined. This model also uses the mist capture technology (e.g. dry filter or waterwash) to determine portions of the oversprayed amount that is released to the air, water, and incineration, or landfill targets.	
EPA/OPPT Automobile Refinish Coating Overspray Loss Model (non-	Daily release=LF x Amt	Automobile <u>Refinish</u> Spray Coating Application
volatile)	Where:	
(used in the Automobile Refinish Spray Coating Operation)	<u>TE=transfer efficiency of the spray gun (25-65%)</u>	
	Amt*=amount of chemical (kg/site-day) to which the loss fraction is applied (e.g., daily amount unloaded from container)	
	*Be sure to read this model's User Guide topic for more information on how the daily amount of chemical is determined.	
	This model also uses the mist capture technology (e.g. dry filter or waterwash) to determine portions of the oversprayed amount that is released to the air, water, and incineration, or landfill targets.	
EPA/OPPT Cooling Tower Blowdown	Daily release=LF x Amt	Recirculating Water-Cooling Tower Additive Releases
LOSS MODEI	Where:	NOTE: This model cannot be chosen as an alternative

(used in the Recirculating Water- Cooling Tower Additive Use operation)	LF=loss fraction; <u>0.6 percent</u> (the loss fraction must be entered and used in the Mass Balance Parameters subtab calculations)	for any other ChemSTEER sources.
	Amt=Daily amount of chemical contained in the recirculating fluid (DRRchem) (kg/site-day) (value must be entered/calculated in the Mass Balance Parameters subtab)	
EPA/OPPT Cooling Tower Windage Loss Model	Daily release=LF x Amt	Recirculating Water-Cooling Tower Additive Releases
(used in the Recirculating Water- Cooling Tower Additive Use operation)	Where: LF=loss fraction; <u>0.1 percent</u> (the loss fraction must be entered and used in the Mass Balance Parameters subtab calculations)	NOTE: This model cannot be chosen as an alternative for any other ChemSTEER sources.
	Amt=Daily amount of chemical contained in the recirculating fluid (DRRchem) (kg/site-day) (value must be entered/calculated in the Mass Balance Parameters subtab)	
EPA/OPPT Cooling Tower Evaporative	Daily release=LF x Amt	Recirculating Water-Cooling Tower Additive Releases
Loss Model	Where.	NOTE: This model cannot be chosen as an alternative
(used in the Recirculating Water- Cooling Tower Additive Use operation)	LF=loss fraction; <u>between 0.5 to 3 percent</u> (the loss fraction must be entered and used in the Mass Balance Parameters subtab calculations)	for any other ChemSTEER sources.
NOTE: this model is only used in cases where the chemical is volatile (i.e., the AVP of the additive is within the specified AVP range)	Amt=Daily amount of chemical contained in the recirculating fluid (DRRchem) (kg/site-day) (value must be entered/calculated in the Mass Balance Parameters subtab)	
EPA/OPPT Electroplating Rinse Water	Daily release*=DVrinse x 3.78 L/gal x Yrinse x Drinse x (1-	Rinsing Electroplated Parts
Loss Model	RinseE)	NOTE: This model cannot be chosen as an alternative
(used in the Electroplating Bath Additive Use operation)	*Be sure to read this model's User Guide topic for more information on how the daily amount of chemical is determined. This model also used the wastewater treatment system efficiency to determine portions of the chemical amount that is released to land or incineration (as sludge) and to water	for any other ChemSTEER sources.

EPA/OPPT Electroplating Spent Bath Disposal Model	Daily release*=DVbath x 3.78 L/gal x Ybath x Dbath	Changing Electroplating Bath
-	*Re sure to read this model's User Guide tonic for more	NOTE: This model cannot be chosen as an alternative
(wood in the Flootnendating Dath	information on how the daily amount of chamical is	for any other Character D sources
(used in the Electropiating Bath	Information on now the daily amount of chemical is	for any other Chemsteer sources.
Additive Use operation)	determined.	
	This model also used the wastewater treatment system	
	efficiency to determine portions of the chemical amount	
	that is released to land or incineration (as sludge) and to	
	water	
Models for Calculating Peleases from Ot	ther Generic Unit Operations to Multi-Media (i.e., air, water, in	cineration and/or landfill)
models for culculating keleases <u>from or</u>	to water, me one operations to water-weata (i.e., all, water, in	
EPA/OPPT Water Saturation Loss Model	Daily release=WSchem x CF x Amt / (1000 g/kg)	Aqueous Wash of Organic Mass
	Where:	
	WSchem=water solubility of the chemical g/L (default:	
	specified in the Chemical tab)	
	specified in the chemical taby	
	CF*=correction factor: default=1	
	Amt*=Amount of water (kg/site-day) in which the chemical	
	is saturated (e.g. mass of water contained in the vessel)	
	is such aced (c.g., mass of water contained in the vessely	
	*Be sure to read this model's User Guide topic for more	
	information on using the correction factor and how the daily	
	amount of water is determined	
	amount of water is determined.	
EPA/OPPT Solids Transfer Dust Model	Daily Release=LF x Amt x SrE	Loading Solids into Transport Containers/Vessels (all
		source types)
	Where:	
	LF=loss fraction; 0.5 percent	Unloading Solids from Transport Containers/Vessels
		(all source types)
	Amt*=amount of chemical (kg/site-day) to which the loss	(
	fraction is applied (a.g., daily amount unleaded from	
	naction is applied (e.g., daily amount unioaded from	
	container)	
	SrE=solids removal efficiency of the control technology (0-	
	0.995)	

	*Be sure to read this model's User Guide topic for more information on how the daily amount of chemical is determined. This model also uses the solids removal efficiency of the control technology (e.g., mechanical collector/cyclone) to determine portions of the amount that is released to air, water, incineration, or landfill targets.	
User-Defined Loss Rate Model	Daily release=LF x Amt	Distillation Column Bottoms Disposal
	Where: LF=loss fraction (you must enter a loss fraction between 0 and 1)	Filter Media Changeout Grinding and Sanding
	Amt*=amount of chemical (kg/site-day) to which the loss fraction is applied (e.g., chemical mass capacity of the vessel)	Liquid/Liquid Extraction Solvent Disposal Scrubber Releases
	*Be sure to read this model's User Guide topic for more information on how the daily amount of chemical is determined.	Roll Coating NOTE: You may choose this model for any source for which you wish to enter a known loss fraction (LF)

# User-Defined Loss Rate Model

# **Model Description**

User-defined loss rate and associated parameters to calculate releases.

# Sources/Activities That Use This Model as a Default

The following sources/activities use the User-Defined Loss Rate Model as the default for calculating releases of a chemical to air, water, incineration, or landfill:

- Distillation Column Bottoms Disposal
- Filter Media Changeout
- Grinding and Sanding
- Liquid/Liquid Extraction Solvent Disposal
- <u>Scrubber Releases</u>
- Roll Coating

This model is appropriate to use as an additional or alternative release model for <u>all</u> other ChemSTEER sources/activities (except the *Recirculating Water-Cooling Tower Additive Releases* source/activity).

# **Potential Media of Release**

Air, Water, Incineration, and/or Landfill (default: 100% of release to water)

# Equations

For daily releases:

DR (kg/site-day) = LF x Amt

DR occurs over [Freq] days/year

For annual releases:

AR (kg/year) = DR x Freq x NS, AR is for all sites combined

# Model Input Parameters and Default Values

The User-Defined Loss Rate Model default values for each of the input parameters are summarized in the table below.

Table A 1. Input Parameters and Default Values for the User-Defined Loss Rate Model

Parameter	Description	Default Value(s)	Units
LF	Loss fraction; fraction of an amount of the chemical that is estimated to be released	User-defined LF	dimensionless
Amt	The amount of chemical to which a loss fraction is applied	Defaults specified in Table A- 1a	kg/site-day
NS	Number of sites	NS (from Mass Balance Parameters subtab of Operation Parameters tab)	site(s)
Freq	The frequency of release of the chemical	Default specified in Table A- 1b	day/site-year
DR	Daily Release rate	Calculated from model equation	kg/site-day
AR	Annual Release rate	Calculated from model equation	kg/year (all sites)

You may elect to change any parameter from Table A- 1 except the model estimates DR and AR. Clicking the *Type* column for each changeable parameter other than LF, Amt and Freq contains only two options: ChemSTEER defaults from Table A- 1 and User-defined. You <u>must</u> enter a value for LF in this release model. The conditional default and non-default options for Amt and Freq are presented in the tables below. Be sure to read the <u>ChemSTEER Estimation Methods and Models</u> topic for more information about changing model parameters.

# Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default Characterization of Output 1 Results: *Output 1* Default Characterization of Output 2 Results: *Output 2* 

You may select an alternative characterization for either of the outputs at any time.

#### **Default Model Basis**

The following default text is displayed in the Basis box on the *View/Update Release Model Information* screen:

"User-Defined Loss Rate Model"

Source/Activity Type/Operation Mode	Batch Condition	Operation Type	Conditional Amt Default (kg/site-day)	Non-default Options for Amt*
Container-Related / Continuous	Not Applicable	Any	For Ncd ≥ 1: MCi x Yi x Ncd (kg chemical/site-day) (from Container Parameters subtab of the Operation Parameters tab) For Ncd < 1: MCi x Yi (kg chemical/container) (from Container Parameters subtab of the Operation Parameters tab)	MCi (kg material/container) MCi x Yi (for Ncd ≥ 1 only) DMIchem DMOchem User-defined Amt
Container-Related / Batch	Any	Any	For Ncd ≥ 1: MCi x Yi x Ncd (kg chemical/site-day) (from Container Parameters subtab of the Operation Parameters tab) For Ncd < 1: MCi x Yi (kg chemical/container) (from Container Parameters subtab of the Operation Parameters tab)	MCi (kg material/container) MCi x Yi (for Ncd ≥ 1 only) BMIchem BMOchem BMIchem x Ls (kg/site-bt) BMOchem x Ls (kg/site-bt) BMIchem x Nbd BMOchem x Nbd BMIchem x Nbd/Ls (kg/line-day) BMOchem x Nbd/Ls
Not Container- Related / Continuous	Not Applicable	Manufacturing	DMOchem (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMIchem User-defined Amt

# Table A-1a. Conditional Default Values for Amt for the User-Defined Loss Rate Model

		Processing	DMIchem (kg/site-day)	DMOchem
		Use	Parameters subtab of the	User-defined Amt
			Operation Parameters	
			tab)	
Not Container-	Number of batches	Manufacturing	BMOchem (kg/line-bt)	BMIchem
Related / Batch	per day		(from Mass Balance	BMIchem x Ls
	(Nbd) < 1		Parameters subtab of the	(kg/site-bt)
	(from Mass Balance Parameters subtab of		tab)	BMOchem x Ls (kg/site-bt)
	the Operation Parameters tab)			User-defined Amt
		Processing	BMIchem (kg/line-bt)	BMIchem
		Use	(from Mass Balance Parameters subtab of the	BMIchem x Ls (kg/site-bt)
			Operation Parameters tab)	BMOchem x Ls (kg/site-bt)
				User-defined Amt
	Number of batches	Manufacturing	BMOchem x Nbd	BMIchem
	per day			BMOchem
	(Nbd) ≥ 1		(from Mass Balance	BMIchem x Nbd
	(from Mass Balance Parameters subtab of the Operation		Parameters subtab of the Operation Parameters tab)	BMIchem x Nbd/Ls (kg/line-day)
	Parameters tab)			BMOchem x Nbd/Ls (kg/line-day)
				User-defined Amt
		Processing	BMIchem x Nbd	BMIchem
		Use	(kg/site-day)	BMOchem
			(from the Mass Balance	BMOchem x Nbd
			Parameters subtab of the Operation Parameters tab)	BMIchem x Nbd/Ls (kg/line-day)
			,	BMOchem x Nbd/Ls (kg/line-day)
				User-defined Amt

\*Non-default options for Amt are available by clicking in the Type column in the View/Update Release Model Information screen in the Releases tab.

Source/Activity Type/Operation Mode	Batch Condition	Conditional Freq Default (days of release/site-yr)	Non-Default Options for Freq*
Container-	Not Applicable	For Ncd ≥ 1:	OD
Related/Continuous		ODa	User-defined Freq
		(from Container Parameters subtab of the Operation Parameters tab)	
		For Ncd < 1:	
		Ncy (containers/site-yr)	
		(from Container Parameters subtab of the Operation Parameters tab)	
Container-	Any	For Ncd ≥ 1:	OD
Related/Batch		ODa	Nby
		(from Container Parameters subtab of the Operation Parameters tab)	User-defined Freq
		For Ncd < 1:	
		Ncy (containers/site-yr)	
		(from Container Parameters subtab of the Operation Parameters tab)	
Not Container-	Not Applicable	OD	User-defined Freq
Related/Continuous		(from Container Parameters subtab of the Operation Parameters tab)	
Not Container-	Number of batches per day	Nby	OD
Related/Batch	(Nbd)<1)	(from Container Parameters	User-defined Freq
	(from Mass Balance Parameters subtab of the Operation Parameters tab)	subtab of the Operation Parameters tab)	
	Number of batches per day	OD	Nby
	(Nbd)≥ 1)	(from Container Parameters	User-defined Freq
	(from Mass Balance Parameters subtab of the Operation Parameters tab)	subtab of the Operation Parameters tab)	

Table A-1b. Conditional Default Values for F	reg for the User-Defined Loss Rate Model
	req for the ober Denned 2000 nate moder

\*Non-default options for Freq are available by clicking in the Type column in the View/Update Release Model Information screen in the Releases tab. Key Rationale for Model

NA

References

NA

Models for Calculating Releases to Air

EPA/OAQPS AP-42 Loading Model

# **Model Description**

This model estimates releases to air from the displacement of air containing chemical vapor as a container/vessel is filled with liquid. This model determines a vapor generation rate (G) based in part upon the chemical's physical-chemical properties and assumes that the rate of evaporation is negligible compared to the loss from displacement.

# Sources/Activities That Use This Model as a Default

The following sources/activities use the EPA/OAQPS AP-42 Loading Model as the default for calculating releases of a volatile chemical to air:

- All sources/activities involving Loading Liquids into Transport Containers/Vessels
- All sources/activities involving <u>Unloading Liquids from Transport Containers/Vessels</u>

(It is assumed that as the container is unloading, another is being loaded. The EPA/OAQPS AP-42 Loading model provides a more conservative estimate of chemical releases that occur during this activity.)

**NOTE:** If the adjusted vapor pressure for the operation (AVPrm or AVPprod) is outside of the preferred AVP range, this model will NOT appear as a default. If the operation AVP is less than the preferred AVPlow (0.001 torr) or greater than the preferred AVPhigh (35 torr), there is no default model for estimating volatile releases to air from these activities. Refer to the <u>Operation</u> <u>Parameters Tab  $\rightarrow$  Shared Parameters/Factors Subtab</u> for more information.

# **Other Sources/Activities**

The EPA/OAQPS AP-42 Loading Model may be an appropriate alternative to the default air release model for the following sources/activities:

- All sources/activities for <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>
- All sources/activities for Equipment Cleaning Losses of Liquids
- Miscellaneous Sources/Activities Related to Liquid Processing
- <u>Aqueous Wash of Organic Mass</u>
- Distillation Column Bottoms Disposal

Liquid/Liquid Extraction Solvent Disposal

#### Mechanism

Displacement of air containing chemical vapor.

#### **Potential Media of Release**

Air, Water, Incineration, and/or Landfill (default: 100% of release to air)

# Equations

For daily releases:

DR (kg/site-day) = (G x 3600 x OHa) / 1000

DR occurs over [Freq] days/year

where:

 $G(g/s) = f \times MW \times (3785.4 \times Vc) \times r \times X \times (VP / 760) / (3600 \times T \times R)$ 

For annual releases:

AR (kg/year) = DR x Freq x NS, AR is for all sites combined

#### **Model Input Parameters and Default Values**

The EPA/OAQPS AP-42 Loading Model default values for each of the input parameters are summarized in Table A-2 below:

Parameter	Description	Default Value(s)	Units
G	Vapor generation rate	Calculated from model equation	g/s
f	Saturation factor	Defaults specified in Table A-2a	dimensionless
MW	Molecular weight of the chemical	MW (from chemical tab)	g/mol
Vc	Volume of the container	VC (from Container Parameter subtab of Operation Parameters tab) Defaults specified in Table A-2a	gallons
r	Fill rate	r (from Container Parameter subtab of Operation Parameters tab) Defaults specified in Table A-2a	containers/hr
Х	Vapor pressure correction factor (mole fraction or other)	Defaults specified in Table A-2b	dimensionless
VP	Vapor pressure of the pure chemical	VP (from chemical tab)	torr
Т	Temperature	298	К
R	Universal Gas Constant	82.05	atm-cm³/gmol- K
ОНа	Operating hours per site-day for the source/activity	Default specified in Table A-2c	hour/site-day
NS	Number of sites	NS (from Mass Balance Parameters subtab of Operation Parameters tab)	site(s)
Freq	The frequency of release of the chemical to a particular medium	Defaults specified in Table A-2d	days/site-year
DR	Daily Release rate	Calculated from model equation	kg/site-day
AR	Annual Release rate	Calculated from model equation	kg/year (all sites)

Table A-2. Input Parameters and Default Values for the EPA/OAQPS AP-42 Loading Model

You may elect to change any parameter from Table A-2 except the model estimates G, DR, and AR. Clicking the *Type* column for each changeable parameter other than X and Freq contains only two options: ChemSTEER defaults from Table A-2 and User-defined. The default values of r, f, and h are dependent upon the selected *source/activity*. These conditional default values are summarized in Table A-2a and Table A-2c. The conditional default and non-default options for X and Freq are also presented in the tables below. Be sure to read the <u>ChemSTEER Estimation Methods and Models</u> topic for more information about changing model parameters.

# Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Enabled* Enable Model Parameters for Output 2: *Enabled* 

Default Characterization of Output 1 Results: Typical

Default Characterization of Output 2 Results: Worst Case

**NOTE:** If you change the default value for either *r* or *f*, the *Characterization of Results* will be automatically reset to Output 1 or Output 2 (as appropriate).

You may select an alternative characterization for either of the outputs at any time.

# **Default Model Basis**

The following default text is displayed in the Basis box on the View/Update Release Model Information screen:

"EPA/OAQPS AP-42 Loading Model"

Vessel Name (Characterization of Parameter Value)	Default Vc (gal)	Range of Volumes (gal)	Default r <sup>1</sup> (containers/hr)	Default f
Bottles		<5		
Output 1 (Typical)	1		60	0.5
Output 2 (Worst Case)	1		60	1
Small Containers		≥ 5 to < 20		
Output 1 (Typical)	5		60	0.5
Output 2 (Worst Case)	5		60	1
Drums		≥ 20 to < 100		
Output 1 (Typical)	55		20	0.5
Output 2 (Worst Case)	55		20	1
Totes		≥ 100 to < 1,000		
Output 1 (Typical)	550		20	0.5
Output 2 (Worst Case)	550		20	1
Tank Truck		≥ 1,000 to < 10,000		
Output 1 (Typical)	5,000		2	1
Output 2 (Worst Case)	5,000		2	1
Rail Car		≥ 10,000		
Output 1 (Typical)	20,000		1	1
Output 2 (Worst Case)	20,000		1	1
User-defined or	User-defined	User-defined	User-defined	
Sources/Activities that are not				
Container-Related				

# Table A-2a. Default Values for Container Volumes (Vc), Fill Rates (r), and Saturation Factors (f) forActivities Involving Liquids

Source: portions from CEB Engineering Manual, USEPA, 1991, Table 4-11.

1. ChemSTEER defaults to the <u>typical</u> container fill rate (r) listed in the background reference document for all vapor generation estimates for container-related sources/activities. The background reference document contains worst case fill rates that would result in higher vapor generation rates; however, these are not used as default values in ChemSTEER. For a fixed total volume of liquid handled, the worst case fill rate would result in a higher generation rate that would occur over a shorter period of time, when compared to that of the typical fill rate (lower generation rate over longer period of time). Thus, with all other parameters being equal, the total annual amount of vapor generated (and resulting releases to air and worker inhalation exposures) are essentially equivalent between the typical and worst case fill rates. For simplicity, ChemSTEER uses the typical fill rate as the default for both Output 1 and Output 2 results. Alternative typical fill rates for smaller containers and bottles were developed as an internal policy decision. The typical rate of 60 containers per hour is the current default; a worst case fill rate of 90 per hour was also decided. The reference document contains the previous defaults of 20 (typical) and 30 (worst case) containers per hour for bottles and small containers; however, these were superseded by this internal policy decision.

Material Named in Source/Activity Label	Operation Type	Conditional X Default	Non-Default Options for X*
Raw Material	Any	Xrm (from Shared Parameters/Factors subtab of the Operation Parameters tab)	Xprod Xother User-defined X
Product	Any	Xprod (from Shared Parameters/Factors subtab of the Operation Parameters tab)	Xrm Xother User-defined X
Other	Any	Xother (from Shared Parameters/Factors subtab of the Operation Parameters tab)	Xrm Xprod User-defined X
Not material-specific	Manufacture	Xprod (from Shared Parameters/Factors subtab of the Operation Parameters tab)	Xrm Xother User-defined X
	Processing Use	Xrm (from Shared Parameters/Factors subtab of the Operation Parameters tab)	Xprod Xother User-defined X

# Table A-2b. Conditional Default Values for X for the EPA/OAQPS AP-42 Loading Model

\*Non-default options for X are available by clicking in the Type column in the View/Update Release Model Information screen in the Releases tab. All default and non-default options for X are available for both Output 1 and Output 2.

# Table A-2c. Conditional Default Values for OHa for the EPA/OAQPS AP-42 Loading Model

Source/Activity Type	Conditional h Default* (hr/site-day)
Container-Related	OHa (from Container Parameters subtab of the Operation Parameters tab)
Sampling	1
Equipment Cleaning Losses of Liquids from Multiple Vessels	4
Equipment Cleaning Losses of Liquids from a Single, Large Vessel	1
Equipment Cleaning Losses of Liquids from a Single, Small Vessel	0.5
Not Container-Related, Sampling, or Equipment Cleaning	8

1. You may select the conditional default h (shown above) or enter a user-defined h for either Output 1 or Output 2. for all sources/activities. The conditional default h values were adopted as a policy decision in 2002.

Source/Activity Type/Operation Mode	Batch Condition	Conditional Freq Default (days of release/site-yr)	Non-Default Options for Freq*
Container- Related/Continuous	Not Applicable	ODa (from Container Parameters subtab of the Operation Parameters tab)	Ncy (Containers/site-yr; from Container Parameters subtab of the Operation Parameters tab)
			OD
			User-defined Freq
Container- Related/Batch	Any	ODa (from Container Parameters subtab of the Operation Parameters tab)	Ncy (Containers/site-yr; from Container Parameters subtab of the Operation Parameters tab) Nby
			OD
			User-defined Freq
Not Container- Related/Continuous	Not Applicable	OD (from Container Parameters subtab of the Operation Parameters tab)	User-defined Freq
Not Container-	Number of batches per day	Nby	OD
Related/Batch	(Nbd)<1) (from Mass Balance Parameters subtab of the Operation Parameters tab)	(from Container Parameters subtab of the Operation Parameters tab)	User-defined Freq
	Number of batches per day	OD	Nby
	(Nbd)≥ 1) (from Mass Balance Parameters subtab of the Operation Parameters tab)	(from Container Parameters subtab of the Operation Parameters tab)	User-defined Freq

### Table A-2d. Conditional Default Values for Freq for the EPA/OAQPS AP-42 Loading Model

\*Non-default options for Freq are available by clicking in the *Type* column in the View/Update Release Model Information screen in the Releases tab. All default and non-default options for Freq are available for both Output 1 and Output 2.

# Key Rationale for Model

As a container/vessel is filled with liquid containing the chemical, some of the chemical in the liquid evaporates into the air in the vessel. The air containing the chemical vapor leaves the vessel at the rate at which the liquid fills the vessel.

# Reference

Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991. (Equation 4-21)

Fehrenbacher, M.C. and Hummel, A.A. "Evaluation of the Mass Balance Model Used by the Environmental Protection Agency for Estimating Inhalation Exposure to New Chemical Substances". *American Industrial Hygiene Association Journal*. June 1996. 57: 526-536.

# EPA/OPPT Mass Transfer Coefficient Model

# **Model Description**

This model estimates releases to air from evaporation of a chemical from an open, exposed liquid surface. This method is the default for select activities that are assumed to be performed outdoors or when air velocities are expected to be greater than 100 feet per minute. This model determines a vapor generation rate (G) based in part upon the chemical's physical-chemical properties and the surface area from which the chemical is evaporating.

# Sources/Activities That Use This Model as a Default

The following sources/activities use the EPA/OPPT Mass Transfer Coefficient Model as the default for calculating releases of a volatile chemical to air:

- Cleaning Liquid Residuals from Tank Trucks Used to Transport the Raw Material/Product (see <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>)
- Cleaning Liquid Residuals from Rail Cars Used to Transport the Raw Material/Product (see <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>)
- All sources/activities involving for <u>Equipment Cleaning Losses of Liquids</u>

**NOTE:** If the adjusted vapor pressure for the operation (AVPrm or AVPprod) is outside of the preferred AVP range, this model will NOT appear as a default. If the operation AVP is less than the preferred AVPlow (0.001 torr) or greater than the preferred AVPhigh (35 torr), there is no default model for estimating volatile releases to air from these activities. Refer to the <u>Operation</u> <u>Parameters Tab  $\rightarrow$  Shared Parameters/Factors Subtab</u> for more information.

# **Other Sources/Activities**

The EPA/OPPT Mass Transfer Model may be an appropriate alternative to the default air release model for the following sources/activities:

Cleaning Liquid Residuals from Transport Containers/Vessels:

- Cleaning Liquid Residuals from Bottles Used to Transport the Raw Material/Product
- Cleaning Liquid Residuals from Small Containers Used to Transport the Raw Material/Product

- Cleaning Liquid Residuals from Drums Used to Transport the Raw Material/Product
- Cleaning Liquid Residuals from Totes Used to Transport the Raw Material/Product
- Cleaning Liquid Residuals from Containers Used to Transport the Raw Material/Product
- Cleaning Liquid Residuals from Storage/Transport Vessels (User-defined)

Unit Operations and Processes:

- Aqueous Wash of Organic Mass
- Filter Media Changeout
- Liquid/Liquid Extraction Solvent Disposal
- <u>Scrubber Releases</u>

# Other Sources/Activities:

- All sources/activities for <u>Sampling Liquids</u>
- All sources/activities for Unloading Liquids from Transport Containers/Vessels
- Miscellaneous Sources/Activities Related to Liquid Processing
- Vapor Releases from Open Liquid Surfaces

### **Roll Coating**

#### Mechanism

Volatilization of the chemical from a static pool.

# Potential Media of Release

Air, Water, Incineration, and/ or Landfill (default: 100% of release to air)

#### Equations

For daily releases:

DR (kg/site-day) = (G x 3600 x OHa) / 1000

DR occurs over [Freq] days/year

where:

For annual releases:

AR (kg/year) = DR x Freq x NS, AR is for all sites combined.

# **Model Input Parameters and Default Values**

The EPA/OPPT Mass Transfer Model input parameters contain several default values that are dependent upon the specific type of activity being assessed. The EPA/OPPT Mass Transfer Model default values for each of the input parameters are summarized in Table A-3:

Table A-3. Equipment Cleaning Activity Input Parameters and Default Values for the EPA/OPPT Mass
Transfer Model

Parameter	Description	Default Value(s)	Units	
G	Vapor generation rate	Calculated from model equation	g/s	
MW	Molecular weight of the chemical	MW (from Chemical tab)	g/mol	
х	Vapor pressure correction factor (mole fraction or other)	Defaults specified in Table A-3a	dimensionless	
VP	Vapor pressure of the pure chemical	VP (from Chemical tab)	torr	
vz	Air speed	440	ft/min	
d	Diameter/length of the static pool or opening	Defaults specified in Table A-3b	ст	
A	Surface area of the static pool or opening	$\pi x d^2/4$	cm <sup>2</sup>	
Т	Temperature	298	К	
ОНа	Operating hours per site-day for the source/activity	Defaults specified in Table A-3b	hours/site-day	
NS	Number of sites	NS (from Mass Balance Parameters subtab of Operation Parameters tab)	site(s)	
Freq	The frequency of release of the chemical to air	Defaults specified in Table A-3c	days/site-year	
DR	Daily release rate	Calculated from model equation	kg/site-day	
AR	Annual release rate	Calculated from model equation	kg/year (all sites)	

You may elect to change any parameter from Table A-3 except the model estimates G, A, DR, and AR. Clicking the *Type* column for each changeable parameter other than X and Freq contains only two options: ChemSTEER defaults from Table A-3 and User-defined. The default values of OHa and d are dependent upon the selected source/activity. These conditional default values are summarized in Table A-3b. The conditional default and non-default options for X and Freq are presented in the tables below. Be sure to read the <u>ChemSTEER Estimation Methods and Models</u> topic for more information about changing model parameters.

If you attempt to use an air speed (vz) less than or equal to 100 ft/min, ChemSTEER will allow you to continue after viewing the following message box:

This model is most appropriate for air speeds greater than 100 ft/min. For air speeds less than or equal to 100 ft/min, you should select and use the EPA/OPPT Penetration Model to estimate the vapor generation rate.@

# Default Parameter Value Switch Settings and Results Characterization

When this model is used by a *liquid sampling* source/activity:

Enable Model Parameters for Output 1: *Enabled* Enable Model Parameters for Output 2: *Enabled* 

When this model is used by *any other* (non-liquid sampling) source/activity:

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default Characterization of Output 1 Results: *Output 1* Default Characterization of Output 2 Results: Output 2 These result characterizations are the default for all sources/activities using the EPA/OPPT Mass Transfer Coefficient Model.

You may select an alternative characterization for either of the outputs at any time.

# **Default Model Basis**

The following default text is displayed in the Basis box on the View/Update Release Model Information screen:

"EPA/OPPT Mass Transfer Coefficient Model"

Material Named in Source/Activity Label	Operation Type	Conditional X Default	Non-Default Options for X*
Raw Material	Any	Xrm (from Shared Parameters/Factors subtab of the Operation Parameters tab)	Xprod Xother User-defined X
Product	Any	Xprod (from Shared Parameters/Factors subtab of the Operation Parameters tab)	Xrm Xother User-defined X
Other	Any	Xother (from Shared Parameters/Factors subtab of the Operation Parameters tab)	Xrm Xprod User-defined X
Not material-specific	Manufacture	Xprod (from Shared Parameters/Factors subtab of the Operation Parameters tab)	Xrm Xother User-defined X
	Processing Use	Xrm (from Shared Parameters/Factors subtab of the Operation Parameters tab)	Xprod Xother User-defined X

# Table A-3a. Conditional Default Values for X for the EPA/OPPT Mass Transfer Model

\*Non-default options for X are available by clicking in the *Type* column in the View/Update Release Model Information screen in the Releases tab. All default and non-default options for X are available for both Output 1 and Output 2.

Source/Activity Type	Default OHa <sup>1</sup> (hrs/site-day)	Default d <sup>2</sup> (cm)
Container-Related	OHa (from Container Parameters subtab of Operation Parameters tab)	5.08 (2-in operating) for Vc < 5,000 gal 7.6 (3-in opening) for Vc ≥ 5,000 gal
Equipment Cleaning Losses of Liquids from Multiple Vessels	4	92 (3-ft manhole)
Equipment Cleaning Losses of Liquids from a Single, Large Vessel	1	92 (3-ft manhole)
Equipment Cleaning Losses of Liquids from a Single, Small Vessel	0.5	92 (3-ft manhole)
Sampling Liquid Product Sampling Liquid Raw Material Sampling Liquids	1	Output 1: <u>Default:</u> 2.5 <sup>3</sup> (Typical) (1-in bottle opening) <u>Non-default options</u> : 10 (Worst Case) and User-defined d <u>Output 2:</u> <u>Default:</u> 10 (Worst Case) (4-in beaker opening) <u>Non-default options</u> : 2.5 <sup>3</sup> (Typical) and User-defined d
All other sources/activities not covered by above for <i>continuous</i> operations	24	User-defined
All other sources/activities not covered by above for <i>batch</i> operations	Lesser of 24 or (HB x Nbd) (from Mass Balance subtab of Operations Parameters tab)	User-defined

# Table A-3b. Default Values for Operation Hours (OHa) and Pool/Opening Diameter (d) for the EPA/OPPT Mass Transfer Model

 You may select the conditional default OHa (shown above) or enter a user-defined OHa for either Output 1 or Output 2 for all sources/activities. The conditional default OHa values were adopted as a policy decision in 2002.
 For non-sampling sources activities, you may select the conditional default d (shown above) or enter a userdefined d for either Output 1 or Output 2.

3. The "typical" diameter default value of 2.5 cm was adopted as a policy decision in 2002, which supersedes the previous default value of 7 cm shown in the 1991 USEPA reference document.

Source/Activity Type/Operation Mode	Batch Condition	Conditional Freq Default (days of release/site-yr)	Non-Default Options for Freq*
Container- Related/Continuous	Not Applicable	ODa (from Container Parameters subtab of the Operation Parameters tab)	Ncy (Containers/site-yr; from Container Parameters subtab of the Operation Parameters tab) OD User-defined Freq
Container- Related/Batch	Any	ODa (from Container Parameters subtab of the Operation Parameters tab)	Ncy (Containers/site-yr; from Container Parameters subtab of the Operation Parameters tab) Nby OD User-defined Freq
Not Container- Related/Continuous	Not Applicable	OD (from Container Parameters subtab of the Operation Parameters tab)	User-defined Freq
Not Container- Related/Batch	Number of batches per day (Nbd)<1) (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby (from Container Parameters subtab of the Operation Parameters tab)	OD User-defined Freq
	Number of batches per day (Nbd)≥ 1) (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD (from Container Parameters subtab of the Operation Parameters tab)	Nby User-defined Freq

Table A-3c. Conditional Defau	t Values for Fred	n for the FPA	<b>/OPPT</b> Mass 1	Fransfer Model
Table A-St. Conditional Delau	L Values IUI ITE			inalister widder

\*Non-default options for Freq are available by clicking in the *Type* column in the View/Update Release Model Information screen in the Releases tab. All default and non-default options for Freq are available for both Output 1 and Output 2.

# Key Rationale for Model

The model is predicated on the solution of the classical mass transfer coefficient model with the gas-phase mass transfer coefficient estimated by the correlation of Mackay and Matsugu. Results were tested against experimental results on 19 compounds generated by four different experimenters over a wide range of experimental conditions. The model matched the experimental data well, usually within 20 percent.

# References

Pre-publication draft article entitled Evaporation of Pure Liquids From Open Surfaces, Fredrick C. Arnold and Alfred J. Engel, US EPA, October, 1999.
Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991.

## EPA/OPPT Penetration Model

#### **Model Description**

This model estimates releases to air from evaporation of a chemical from an open, exposed liquid surface. This method is the default for select activities that are assumed to be performed indoors or when air velocities are expected to be less than or equal to 100 feet per minute. This model determines a vapor generation rate (G) based in part upon the chemical's physical-chemical properties and the surface area from which the chemical is evaporating.

#### Sources/Activities That Use This Model as a Default

The following sources/activities use the EPA/OPPT Penetration Model as the default for calculating releases of a volatile chemical to air:

- Cleaning Liquid Residuals from Bottles Used to Transport the Raw Material/Product (see <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>)
- Cleaning Liquid Residuals from Small Containers Used to Transport the Raw Material/Product (see <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>)
- Cleaning Liquid Residuals from Drums Used to Transport the Raw Material/Product (see <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>)
- Cleaning Liquid Residuals from Totes Used to Transport the Raw Material/Product (see <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>)
- Cleaning Liquid Residuals from Storage/Transport Vessels (User-defined) (see <u>Cleaning</u> Liquid Residuals from Transport Containers/Vessels)
- All sources/activities for <u>Sampling Liquids</u>

**NOTE:** If the adjusted vapor pressure for the operation (AVPrm or AVPprod) is outside of the preferred AVP range, this model will NOT appear as a default. If the operation AVP is less than the preferred AVPlow (0.001 torr) or greater than the preferred AVPhigh (35 torr), there is no default model for estimating volatile releases to air from these activities. Refer to the <u>Operation</u> <u>Parameters Tab  $\rightarrow$  Shared Parameters/Factors Subtab</u> for more information.

## **Other Sources/Activities**

The EPA/OPPT Penetration Model may be an appropriate alternative to the default air release model for the following sources/activities:

Cleaning Liquid Residuals from Transport Containers/Vessels:

- Cleaning Liquid Residuals from Tank Trucks Used to Transport the Raw Material/Product
- Cleaning Liquid Residuals from Rail Cars Used to Transport the Raw Material/Product

• Cleaning Liquid Residuals from Containers Used to Transport the Raw Material/Product

#### Unit Operations and Processes:

- Aqueous Wash of Organic Mass
- Filter Media Changeout
- Liquid/Liquid Extraction Solvent Disposal
- <u>Scrubber Releases</u>

Other Sources/Activities:

- All sources/activities for <u>Sampling Liquids</u>
- All sources/activities for <u>Unloading Liquids from Transport Containers/Vessels</u>
- Miscellaneous Sources/Activities Related to Liquid Processing
- Vapor Releases from Open Liquid Surfaces

#### **Roll Coating**

#### Mechanism

Volatilization of the chemical from a static pool.

#### **Potential Media of Release**

Air, Water, Incineration, and/ or Landfill (default: 100% of release to air)

#### Equations

For daily releases:

 $DR (kg/site-day) = (G \times 3600 \times OHa) / 1000$ 

DR occurs over [Freq] days/year

where:

For annual releases:

AR (kg/year) = DR x Freq x NS, AR is for all sites combined

#### Model Input Parameters and Default Values

The EPA/OPPT Penetration Model input parameters contain several default values that are dependent upon the specific type of activity being assessed. The EPA/OPPT Penetration Model default values for each of the input parameters are summarized in Table A-4:

Parameter	Description	Default Value(s)	Units
G	Vapor generation rate	Calculated from model equation	g/s
MW	Molecular weight of the chemical	MW (from Chemical tab)	g/mol
х	Vapor pressure correction factor (mole fraction or other)	Defaults specified in Table A-4a	dimensionless
VP	Vapor pressure of the pure chemical	VP (from Chemical tab)	torr
vz	Air speed	100	ft/min
d	Diameter/length of the static pool or opening	Defaults specified in Table A-4b	ст
A	Surface area of the static pool or opening	$\pi x d^2/4$	cm <sup>2</sup>
Т	Temperature	298	К
Р	Ambient atmospheric pressure	1	atm
ОНа	Operating hours per site-day for the source/activity	Defaults specified in Table A-4b	hours/site-day
NS	Number of sites	NS (from Mass Balance Parameters subtab of Operation Parameters tab)	site(s)
Freq	The frequency of release of the chemical to air	Defaults specified in Table A-4c	days/site-year
DR	Daily release rate	Calculated from model equation	kg/site-day
AR	Annual release rate	Calculated from model equation	kg/year (all sites)

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1 abie A-4. III	put Parameters	and Default	values for the	EFA/OFFI	renetration	would

You may elect to change any parameter from Table A-4 except the model estimates G, A, DR, and AR. Clicking the *Type* column for each changeable parameter other than X and Freq contains only two options: ChemSTEER defaults from Table A-4 and User-defined. The default values of OHa and d are dependent upon the selected source/activity. These conditional default values are summarized in Table A-4b. The conditional default and non-default options for X and Freq are presented in the tables below. Be sure to read the <u>ChemSTEER Estimation Methods and Models</u> topic for more information about changing model parameters.

If you attempt to use an air speed greater than 100 ft/min, ChemSTEER will allow you to continue after viewing the following message box:

"This model is most appropriate for air speeds less than or equal to 100 ft/min. For air speeds greater than 100 ft/min, you should select and use the EPA/OPPT Mass Transfer Model to estimate the vapor generation rate."

#### Default Parameter Value Switch Settings and Results Characterization

When this model is used by a *liquid sampling* source/activity:

Enable Model Parameters for Output 1: *Enabled* Enable Model Parameters for Output 2: *Enabled* 

Settings for either Output 1 or Output 2 results for liquid sampling sources/activities are based on which default diameter (d) is selected for the corresponding output (refer to Table A-4b below):

- Results using the high end diameter (10 cm) are characterized as Worst-Case by default.
- Results using the typical diameter (2.5 cm) are characterized as Typical by default.
- If you enter a user-defined diameter, the results are characterized as Output 1 or Output2, as appropriate.

When this model is used by *any other* (non-liquid sampling) source/activity:

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default Characterization of Output 1 Results: *Output 1* Default Characterization of Output 2 Results: *Output 2* 

You may select an alternative characterization for either of the outputs at any time.

#### **Default Model Basis**

The following default text is displayed in the Basis box on the *View/Update Release Model Information* screen:

"EPA/OPPT Penetration Model"

Material Named in Source/Activity Label	Operation Type	Conditional X Default	Non-Default Options for X*
Raw Material	Any	Xrm (from Shared Parameters/Factors subtab of the Operation Parameters tab)	Xprod Xother User-defined X
Product	Any	Xprod (from Shared Parameters/Factors subtab of the Operation Parameters tab)	Xrm Xother User-defined X
Other	Any	Xother (from Shared Parameters/Factors subtab of the Operation Parameters tab)	Xrm Xprod User-defined X
Not material-specific	Manufacture	Xprod (from Shared Parameters/Factors subtab of the Operation Parameters tab)	Xrm Xother User-defined X
	Processing Use	Xrm (from Shared Parameters/Factors subtab of the Operation Parameters tab)	Xprod Xother User-defined X

#### Table A-4a. Conditional Default Values for X for the EPA/OPPT Penetration Model

\*Non-default options for X are available by clicking in the Type column in the View/Update Release Model Information screen in the Releases tab. All default and non-default options for X are available for both Output 1 and Output 2.

Source/Activity Type	Default OHa <sup>1</sup> (hrs/site-day)	Default d <sup>2</sup> (cm)
Container-Related	OHa (from Container Parameters subtab of Operation Parameters tab)	5.08 (2-in operating) for Vc < 5,000 gal 7.6 (3-in opening) for Vc ≥ 5,000 gal
Equipment Cleaning Losses of Liquids from Multiple Vessels	4	92 (3-ft manhole)
Equipment Cleaning Losses of Liquids from a Single, Large Vessel	1	92 (3-ft manhole)
Equipment Cleaning Losses of Liquids from a Single, Small Vessel	0.5	92 (3-ft manhole)
Sampling Liquid Product Sampling Liquid Raw Material Sampling Liquids	1	Output 1: <u>Default:</u> 2.5 <sup>3</sup> (Typical) (1-in bottle opening) <u>Non-default options</u> : 10 (Worst Case) and User-defined d <u>Output 2:</u> <u>Default:</u> 10 (Worst Case) (4-in beaker opening) <u>Non-default options</u> : 2.5 <sup>3</sup> (Typical) and User-defined d
All other sources/activities not covered by above for <i>continuous</i> operations	24	User-defined
All other sources/activities not covered by above for <i>batch</i> operations	Lesser of 24 or (HB x Nbd) (from Mass Balance subtab of Operations Parameters tab)	User-defined

# Table A-4b. Default Values for Operation Hours (OHa) and Pool/Opening Diameter (d) for the EPA/OPPT Penetration Model

 You may select the conditional default OHa (shown above) or enter a user-defined OHa for either Output 1 or Output 2 for all sources/activities. The conditional default OHa values were adopted as a policy decision in 2002.
 For non-sampling sources activities, you may select the conditional default d (shown above) or enter a userdefined d for either Output 1 or Output 2.

3. The "typical" diameter default value of 2.5 cm was adopted as a policy decision in 2002, which supersedes the previous default value of 7 cm shown in the 1991 USEPA reference document.

Source/Activity Type/Operation Mode	Batch Condition	Conditional Freq Default (days of release/site-yr)	Non-Default Options for Freq*
Container- Related/Continuous	Not Applicable	ODa (from Container Parameters subtab of the Operation Parameters tab)	Ncy (Containers/site-yr; from Container Parameters subtab of the Operation Parameters tab) OD User-defined Freq
Container- Related/Batch	Any	ODa (from Container Parameters subtab of the Operation Parameters tab)	Ncy (Containers/site-yr; from Container Parameters subtab of the Operation Parameters tab) Nby OD User-defined Freq
Not Container- Related/Continuous	Not Applicable	OD (from Container Parameters subtab of the Operation Parameters tab)	User-defined Freq
Not Container- Related/Batch	Number of batches per day (Nbd)<1) (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby (from Container Parameters subtab of the Operation Parameters tab)	OD User-defined Freq
	Number of batches per day (Nbd)≥ 1) (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD (from Container Parameters subtab of the Operation Parameters tab)	Nby User-defined Freq

#### Table A-4c. Conditional Default Values for Freq for the EPA/OPPT Penetration Model

\*Non-default options for Freq are available by clicking in the Type column in the View/Update Release Model Information screen in the Releases tab. All default and non-default options for Freq are available for both Output 1 and Output 2.

## Key Rationale for Model

The model was developed using Fick's second law of diffusion. Model results were tested against experimental results of a study on evaporation rates for 15 compounds studied at different air velocities and temperatures in a test chamber. The experimental data confirmed the utility and accuracy of the model equation.

#### Reference

Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991. (Equation 4-24 and Appendix K) Fehrenbacher, M.C. and Hummel, A.A. "Evaluation of the Mass Balance Model Used by the References Environmental Protection Agency for Estimating Inhalation Exposure to New Chemical Substances". American Industrial Hygiene Association Journal. June 1996. 57: 526-536.

#### EPA/OPPT Cooling Tower Windage Loss Model

#### **Model Description**

This model estimates releases of a cooling tower additive chemical as a result of windage losses of the recirculating fluid (e.g., water). This model assumes that 0.1 percent of the cooling tower's recirculation rate is lost due to windage.

NOTE: This model is a default model for estimating releases to air from the <u>Recirculating Water-</u> <u>Cooling Tower Additives</u> source/ activity. This model may not be used for any other source/ activity in ChemSTEER.

#### **Potential Media of Release**

Air, Incineration, Landfill and/or Water (default: 100% release to air)

#### Equations

For daily releases:

DR (kg/site-day) = LF × Amt

DR occurs over [Freq] days/year

For annual releases:

AR (kg/year) = DR × Freq × NS, AR is for all sites combined

#### **Model Input Parameters and Default Values**

The EPA/OPPT Cooling Tower Windage Loss Model default values for each of the input parameters are summarized in Table A-5.

Parameter	Description	Default Value(s)	Units
LF	Loss fraction; fraction of an amount of the chemical that is estimated to be released	Value of LFw from Mass Balance subtab Daily Mass of Chemical Used (DMUchem) screen; ChemSteer default for LFw is 0.001	dimensionless
Amt	The amount of chemical to which a loss fraction is applied	Value of DRRchem from Mass Balance subtab Daily Mass of Chemical Used (DMUchem) screen	kg/site-day
Freq	The frequency of release of the chemical	OD (from Mass Balance Parameters subtab of Operation Parameters tab)	day/site-year
NS	Number of sites	NS (from Mass Balance Parameters subtab of Operation Parameters tab)	site(s)
DR	Total daily release rate of tower blowdown	Calculated from model equation	kg/site-day
AR	Total annual release rate of tower blowdown	Calculated from model equation	kg/year (all sites)

#### Table A-5. Input Parameters and Default Values for the EPA/OPPT Cooling Tower Windage Loss Model

You may not change any parameter from Table A-5.

#### Default Parameter Value Switch Settings and Results Characterization:

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default characterizations for either Output 1 or Output 2 results are What-if.

You may select an alternative characterization for either of the outputs at any time.

#### **Default Model Basis**

The following default text is displayed in the Basis box on the *View/Update Release Model Information* screen:

"EPA/OPPT Cooling Tower Windage Loss Model; up to 0.1% of the tower recirculation rate"

#### **Key Rationale for Model**

Windage losses are a function of the mist eliminator design and generally range from less than 0.1% up to 0.2% of the tower's recirculation rate. Some cooling tower manufacturers warrant as low as 0.008% for windage losses. In the absence of other information, this model assumes as a default that 0.1% of the tower's recirculation rate.

#### Reference

Summary Sheet: Recirculating Water-Cooling Tower, No date.

# EPA/OPPT Cooling Tower Evaporative Loss Model (volatiles)

#### **Model Description**

This model estimates releases of a volatile cooling tower additive chemical as a result of evaporation of the recirculating fluid (e.g., water). This model assumes that a user-specified fraction of the cooling tower's recirculation rate is lost due to evaporation.

**NOTE**: This model is a conditional default model for estimating releases to air from the <u>Recirculating Water-Cooling Tower Additives</u> source/activity when the vapor pressure of the chemical (VP) from the Chemical tab is above the low end of the range of adjusted vapor pressure for the operation (AVPlow). If the vapor pressure of the chemical (VP) from the Chemical tab is below the low end of the range of adjusted vapor pressure for the operation (AVPlow). If the vapor pressure of the chemical (VP) from the Chemical tab is below the low end of the range of adjusted vapor pressure for the operation (AVPlow), this model will NOT appear as a default because evaporative releases to air from the cooling tower are assumed negligible for non-volatiles. Refer to <u>Operation Parameters Tab  $\rightarrow$  Shared Parameters/Factors Subtab</u>for more information.

This model may not be used for any other source/activity in ChemSTEER.

#### Potential Media of Release

Air, Incineration, Landfill and/or Water (default: 100% release to air)

#### Equations

For daily releases:

DR (kg/site-day) = LF × Amt

DR occurs over [Freq] days/year

For annual releases:

AR (kg/year) = DR × Freq × NS, AR is for all sites combined

## **Model Input Parameters and Default Values**

The EPA/OPPT Cooling Tower Evaporative Loss Model (volatiles) default values for each of the input parameters are summarized in Table A-6.

# Table A-6. Input Parameters and Default Values for the EPA/OPPT Cooling Tower Evaporative Loss Model (volatiles)

Parameter	Description	Default Value(s)	Units
LF	Loss fraction; fraction of an amount of the chemical that is estimated to be released	Value of LFe from Mass Balance subtab <i>Daily</i> <i>Mass of Chemical Used (DMUchem)</i> screen; ChemSTEER default for LFw is 0	dimensionless
Amt	The amount of chemical to which a loss fraction is applied	Value of DRRchem from Mass Balance subtab <i>Daily Mass of Chemical Used (DMUchem)</i> screen ChemSTEER default for DRRchem is 10,900	kg/site-day
Freq	The frequency of release of the	OD	day/site-year

	chemical	(from Mass Balance Parameters subtab of Operation Parameters tab)	
NS	Number of sites	NS (from Mass Balance Parameters subtab of Operation Parameters tab)	site(s)
DR	Total daily release rate of tower blowdown	Calculated from model equation	kg/site-day
AR	Total annual release rate of tower blowdown	Calculated from model equation	kg/year (all sites)

You may not change any parameter from Table A-6. If the assessed chemical has significant volatility and you determine that a non-zero volatility is appropriate, you should change the value of LFe in Mass Balance subtab *Daily Mass of Chemical Used (DMUchem)* screen.

#### Default Parameter Value Switch Settings and Results Characterization:

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default characterizations for either Output 1 or Output 2 results are What-if.

You may select an alternative characterization for either of the outputs at any time.

#### **Default Model Basis**

The following default text is displayed in the Basis box on the *View/Update Release Model Information* screen:

"EPA/OPPT Cooling Tower Evaporative Loss Model (volatiles); user-specified fraction of the tower recirculation rate"

#### **Key Rationale for Model**

Evaporative losses typically range from 0.5 to 3 percent of the cooling tower's capacity. If the component within the evaporating fluid is non-volatile, the losses of that component to evaporation are expected to be negligible. ChemSTEER defaults to a zero loss rate regardless of volatility. There is no method for determining the relationship between volatility and evaporative loss. If the assessed chemical has significant volatility, the user should make a judgment as to whether a non-zero volatility is appropriate.

#### Reference

Summary Sheet: Recirculating Water-Cooling Tower, No date.

## User-Defined Vapor Generation Rate Model

#### **Model Description**

User-defined vapor generation rate and associated parameters.

#### Sources/Activities That Use This Model as a Default

The User-Defined Vapor Generation Model is the default for calculating releases of a volatile chemical to air for the <u>Vapor Releases from Open Liquid Surfaces</u>.

#### **Other Sources/Activities**

The User-Defined Vapor Generation Rate Model may also be an appropriate means to calculate volatile releases of the chemical from the following sources/activities:

- All sources/activities for <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>
- All sources/activities for Equipment Cleaning Losses of Liquids
- All sources/activities for Loading Liquids into Transport Containers/Vessels
- All sources/activities for <u>Unloading Liquids from Transport Containers/Vessels</u>
- All <u>Generic Coating Applications</u> sources/activities
- All <u>Automobile Spray Coating</u> sources/activities
- Miscellaneous Sources/Activities Related to Liquid Processing
- Vapor Releases from Open Liquid Surfaces

Unit Operations and Processes:

- Aqueous Wash of Organic Mass
- Distillation Column Bottoms Disposal
- Filter Media Changeout
- Liquid/Liquid Extraction Solvent Disposal

Scrubber Releases

#### **Potential Media of Release**

Air, Water, Incineration, and/ or Landfill (default: 100% of release to air)

#### Equations

For daily releases:

DR (kg/site-day) = (G x 3600 x OHa) / 1000

DR occurs over [Freq] days/year

For annual releases:

AR (kg/year) = DR x Freq x NS, AR is for all sites combined

## Model Input Parameters and Default Values

The User-Defined Vapor Generation Rate Model default values for each of the input parameters are summarized in Table A-7.

Parameter	Description	Default Value(s)	Units
G	Vapor generation rate	User-defined G	g/s
ОНа	Operating hours per site-day for the activity	Defaults specified in Table A-7a	hours/site-day
NS	Number of sites	NS (from Mass Balance Parameters subtab of Operation Parameters tab)	site(s)
Freq	The frequency of release of the chemical	Default specified in Table A-7b	day/site-year
DR	Daily Release rate	Calculated from model equation	kg/site-day
AR	Annual Release rate	Calculated from model equation	kg/year (all sites)

Table A-7. Input Parameters for the User-Defined Vapor Generation Rate Model

You may elect to change any parameter from Table A-7 except the model estimates DR and AR. Clicking the *Type* column for each changeable parameter other than G and Freq contains only two options: ChemSTEER defaults from Table A-7 and User-defined. You <u>must</u> enter a value for G in this release model. The default value of OHa is dependent upon the selected source/activity. These conditional default values are summarized in Table A-7a. The conditional default and non-default options for Freq are presented in Table A-7b below. Be sure to read the <u>ChemSTEER Estimation Methods</u> and <u>Models</u> topic for more information about changing model parameters.

#### Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default Characterization of Output 1 Results: *Output 1* Default Characterization of Output 2 Results: *Output 2* 

You may select an alternative characterization for either of the outputs at any time.

#### **Default Model Basis**

The following default text is displayed in the Basis box on the *View/Update Release Model Information* screen:

"User-defined Vapor Generation Rate Model"

Source/Activity Type	Default OHa <sup>1</sup> (hrs/site-day)			
Container-Related	OHa (from Container Parameters subtab of the Operation Parameters tab)			
Equipment Cleaning Losses of Liquids from Multiple Vessels	4			
Equipment Cleaning Losses of Liquids from a Single, Large Vessel	1			
Equipment Cleaning Losses of Liquids from a Single, Small Vessel	0.5			
Sampling Liquid Product, Sampling Liquid Raw Material, Sampling Liquids	1			
All other sources/activities not covered by above for <i>continuous</i> operations	24			
All other sources/activities not covered by above for <i>batch</i> operations	Less of 24 or (HB x Nbd) (from Mass Balance subtab of the Operations Parameters tab)			

Table A-7a. Default Values for Operation Hours (OHa) for the User-Defined Vapor Generation RateModel

1. You may select the conditional default OHa (shown above) or enter a user-defined OHa for either Output 1 or Output 2 for all sources/activities. The conditional default OHa values were adopted as a policy decision in 2002.

Source/Activity Type/Operation Mode	Batch Condition	Conditional Freq Default (days of release/site-yr)	Non-Default Options for Freq*
Container- Related/Continuous	Not Applicable	ODa (from Container Parameters subtab of the Operation Parameters tab)	Ncy (Containers/site-yr; from Container Parameters subtab of the Operation Parameters tab) OD User-defined Freq
Container- Related/Batch	Any	ODa (from Container Parameters subtab of the Operation Parameters tab)	Ncy (Containers/site-yr; from Container Parameters subtab of the Operation Parameters tab) Nby OD User-defined Freq
Not Container- Related/Continuous	Not Applicable	OD (from Container Parameters subtab of the Operation Parameters tab)	User-defined Freq
Not Container- Related/Batch	Number of batches per day (Nbd)<1) (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby (from Container Parameters subtab of the Operation Parameters tab)	OD User-defined Freq
	Number of batches per day (Nbd)≥ 1) (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD (from Container Parameters subtab of the Operation Parameters tab)	Nby User-defined Freq

# Table A-7b. Conditional Default Values for Freq for the User-Defined Vapor Generation Rate Model

\*Non-default options for Freq are available by clicking in the Type column in the View/Update Release Model Information screen in the Releases tab.

#### Key Rationale for Model

NA

Reference

NA

Models for Calculating Releases to Other Media

EPA/OPPT Bulk Transport Residual Model

**Model Description** 

EPA assumes that liquids are pumped from bulk transport containers and that up to 0.2% (a central tendency of 0.07%) of the liquid originally in the bulk container remains as residual after unloading.

#### Sources/Activities That Use This Model as a Default

The following sources/activities use the EPA/OPPT Bulk Transport Residual Model as the default non-air releases model:

- Cleaning Liquid Residuals from Totes Used to Transport the Raw Material/Product (see <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>)
- Cleaning Liquid Residuals from Tank Trucks Used to Transport the Raw Material/Product (see <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>)
- Cleaning Liquid Residuals from Rail Cars Used to Transport the Raw Material/Product (see <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>)

#### **Other Sources/Activities**

The EPA/OPPT Bulk Transport Residual Model may be an appropriate alternative to the default non-air release model for the following sources/activities:

- Cleaning Liquid Residuals from Containers Used to Transport the Raw Material/Product (see <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>)
- Cleaning Liquid Residuals from Storage/Transport Vessels (User-defined) (see <u>Cleaning</u> Liquid Residuals from Transport Containers/Vessels)

#### **Potential Media of Release**

Water, Incineration, and/ or Landfill (default: 100% of release to water)

#### Equations

For daily releases:

DR (kg/site-day) = LF x Amt

DR occurs over [Freq] days/year

For annual releases:

AR (kg/year) = DR x Freq x NS, AR is for all sites combined

#### Model Input Parameters and Default Values

The EPA/OPPT Bulk Transport Residual Model default values for each of the input parameters are summarized in Table A-8.

Parameter	Description	Default Value(s)	Units
LF	Loss fraction; fraction of an amount of the chemical that is estimated to be released	Output 1: <u>Default:</u> 0.0007 (Central Tendency) <u>Non-default option:</u> 0.002 (High End) Output 2: <u>Default:</u> 0.002 (High End) <u>Non-default option:</u> 0.0007 (Central Tendency)	dimensionless
Amt	The amount of chemical to which a loss fraction is applied	Defaults specified in Table A-8a	kg/site-day
NS	Number of sites	NS (from Mass Balance Parameters subtab of Operation Parameters tab)	site(s)
Freq	The frequency of release of the chemical	Default specified in Table A-8b	day/site-year
DR	Daily Release rate	Calculated from model equation	kg/site-day
AR	Annual Release rate	Calculated from model equation	kg/year (all sites)

#### Table A-8. Input Parameters and Default Values for the EPA/OPPT Bulk Transport Residual Model

You may elect to change any parameter from Table A-8 except the model estimates DR and AR. Clicking the *Type* column for each changeable parameter other than LF, Amt and Freq contains only two options: ChemSTEER defaults from Table A-8 and User-defined. The conditional default and non-default options for Amt and Freq are presented in the tables below. Be sure to read the <u>ChemSTEER Estimation</u> <u>Methods and Models</u> topic for more information about changing model parameters.

You may not change the defining model parameter, LF, to be anything other than one of the defaults shown above. If you wish to model releases from bulk container residues using your own loss fraction, choose the <u>User-Defined Loss Rate Model</u>.

#### Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Settings for either Output 1 or Output 2 results are based on which LF is selected for the corresponding output:

- Results using the high end loss fraction are characterized as *High End* by default.
- Results using the central tendency loss fraction are characterized as *Central Tendency* by default.

#### **Default Model Basis**

The following default text is displayed in the Basis box on the *View/Update Release Model Information* screen:

"EPA/OPPT Bulk Transport Residual Model, CEB standard 0.2% residual"

Source/Activity Type/Operation Mode	Batch Condition	Operation Type	Conditional Amt Default (kg/site-day)	Non-default Options for Amt*
Container-Related / Continuous	Not Applicable	Any	For Ncd ≥ 1: MCi x Yi x Ncd (kg chemical/site-day) (from Container Parameters subtab of the Operation Parameters tab) For Ncd < 1:	MCi (kg material/container) MCi x Yi (for Ncd ≥ 1 only) DMIchem DMOchem User-defined Amt
			MCi x Yi (kg chemical/container) (from Container Parameters subtab of the Operation Parameters tab)	
Container-Related / Batch	Any	Any	For Ncd ≥ 1: MCi x Yi x Ncd (kg chemical/site-day) (from Container Parameters subtab of the Operation Parameters tab)	MCi (kg material/container) MCi x Yi (for Ncd ≥ 1 only) BMIchem BMOchem BMIchem x Ls
			For Ncd < 1: MCi x Yi (kg chemical/container) (from Container Parameters subtab of the Operation Parameters tab)	(kg/site-bt) BMOchem x Ls (kg/site-bt) BMIchem x Nbd BMOchem x Nbd/Ls (kg/line-day) BMOchem x Nbd/Ls (kg/line-day) User-defined Amt
Not Container- Related / Continuous	Not Applicable	Manufacturing	DMOchem (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMIchem User-defined Amt
		Processing Use	DMIchem (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMOchem User-defined Amt
Not Container- Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab	Manufacturing	BMOchem (kg/line-bt) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMIchem x Ls (kg/site-bt) BMOchem x Ls (kg/site-bt)

# Table A-8a. Conditional Default Values for Amt for the EPA/OPPT Bulk Transport Residual Model

of the Operation			User-defined Amt
Parameters tab)	Processing Use	BMIchem (kg/line-bt) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMIchem x Ls (kg/site-bt) BMOchem x Ls (kg/site-bt) User-defined Amt
Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Manufacturing	BMOchem x Nbd (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMOchem BMIchem x Nbd BMIchem x Nbd/Ls (kg/line-day) BMOchem x Nbd/Ls (kg/line-day) User-defined Amt
	Processing Use	BMIchem x Nbd (kg/site-day) (from the Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMOchem BMOchem x Nbd BMIchem x Nbd/Ls (kg/line-day) BMOchem x Nbd/Ls (kg/line-day) User-defined Amt

\*Non-default options for Amt are available by clicking in the Type column in the View/Update Release Model Information screen in the Releases tab.

Source/Activity Type/Operation Mode	Batch Condition	Conditional Freq Default (days of release/site-yr)	Non-Default Options for Freq*
Container-	Not Applicable	For Ncd ≥ 1:	OD
Related/Continuous		ODa	User-defined Freq
		(from Container Parameters subtab of the Operation Parameters tab)	
		For Ncd < 1:	
		Ncy (containers/site-yr)	
		(from Container Parameters subtab of the Operation Parameters tab)	
Container-	Any	For Ncd ≥ 1:	OD
Related/Batch		ODa	Nby
		(from Container Parameters subtab of the Operation Parameters tab)	User-defined Freq
		For Ncd < 1:	
		Ncy (containers/site-yr)	
		(from Container Parameters subtab of the Operation Parameters tab)	
Not Container-	Not Applicable	OD	User-defined Freq
Related/Continuous		(from Container Parameters subtab of the Operation Parameters tab)	
Not Container-	Number of batches per day	Nby	OD
Related/Batch	(Nbd)<1)	(from Container Parameters	User-defined Freq
	(from Mass Balance Parameters subtab of the Operation Parameters tab)	subtab of the Operation Parameters tab)	
	Number of batches per day	OD	Nby
	(Nbd)≥ 1)	(from Container Parameters	User-defined Freq
	(from Mass Balance Parameters subtab of the Operation Parameters tab)	subtab of the Operation Parameters tab)	

# Table A-8b. Conditional Default Values for Freq for the EPA/OPPT Bulk Transport Residual Model

\*Non-default options for Freq are available by clicking in the Type column in the View/Update Release Model Information screen in the Releases tab.

#### Key Rationale for Model

The two tenths and seven hundredths of one percent loss are high-end and central tendency values, respectively, in a range of values from an EPA-sponsored study of liquid residuals in bottom-unloaded, gravity drain tanks.

#### References

US EPA Memo entitled Standard Assumptions for PMN Assessments from the Chemical Engineering Branch Quality Panel to Chemical Engineering Branch Staff and Management. 10/92.

PEI Associates for US EPA/OTS. Releases During Cleaning of Equipment. July 1988.

# EPA/OPPT Drum Residual Model

#### Model Description

EPA assumes that liquids are pumped from drums and that up to 3% (a central tendency of 2.5%) of the liquid originally in the drums remains as residual after unloading. Alternative assumptions include 0.6% high end and 0.3% central tendency when pouring liquids from drums.

#### Sources/Activities That Use This Model as a Default

The following sources/activities use the EPA/OPPT Drum Residual Model as the default non-air release model:

- Cleaning Liquid Residuals from Drums Used to Transport the Raw Material/Product (see <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>)
- Cleaning Liquid Residuals from Containers Used to Transport the Raw Material/Product (see <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>)
- Cleaning Liquid Residuals from Storage/Transport Vessels (User-defined) (see <u>Cleaning</u> <u>Liquid Residuals from Transport Containers/Vessels</u>)

## **Other Sources/Activities**

The EPA/OPPT Drum Residual Model may be an appropriate alternative to the default non-air release model for the following sources/activities:

- Cleaning Liquid Residuals from Bottles Used to Transport the Raw Material/Product (see <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>)
- Cleaning Liquid Residuals from Small Containers Used to Transport the Raw Material/Product (see <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>)
- Cleaning Liquid Residuals from Totes Used to Transport the Raw Material/Product (see <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>)

#### **Potential Media of Release**

Water, Incineration, and/ or Landfill (default: 100% of release to water)

**NOTE**: a 1994 policy decision was issued to account for uncertainties in media of releases, and many residual releases are assumed to be released to water as a default. This 1994 decision supersedes the default medium of release that is listed in the 1992 reference memorandum.

#### Equations

For daily releases:

DR (kg/site-day) = LF × Amt

DR occurs over [Freq] days/year

For annual releases:

AR (kg/year) = DR × Freq × NS, AR is for all sites combined

#### **Model Input Parameters and Default Values**

The EPA/OPPT Drum Residual Model default values for each of the input parameters are summarized in Table A-9.

Parameter	Description	Default Value(s)	Units
LF	Loss fraction; fraction of an amount of the chemical that is estimated to be released	Output 1: <u>Default:</u> 0.025 (Central Tendency) <u>Non-default option:</u> 0.03 (High End)*; 0.006 (High End for pouring); and 0.003 (Central Tendency for pouring)	dimensionless
		Output 2: <u>Default:</u> 0.03 (High End for pumping)* <u>Non-default option:</u> 0.025 (Central Tendency); 0.006 (High End for pouring); and 0.003 (Central Tendency for pouring)	
Amt	The amount of chemical to which a loss fraction is applied	Defaults specified in Table A-9a	kg/site-day
NS	Number of sites	NS (from Mass Balance Parameters subtab of Operation Parameters tab)	site(s)
Freq	The frequency of release of the chemical	Default specified in Table A-9b	day/site-year
DR	Daily Release rate	Calculated from model equation	kg/site-day
AR	Annual Release rate	Calculated from model equation	kg/year (all sites)

#### Table A-9. Input Parameters and Default Values for the EPA/OPPT Drum Residual Model

\*The high end loss fraction (LF) was developed as an internal policy decision in 2002. The 1992 EPA memorandum reference document contains the previous default of 4 percent (high end for pumping); however, this was superseded by this internal policy decision.

You may elect to change any parameter from Table A-9 except the model estimates DR and AR. Clicking the *Type* column for each changeable parameter other than LF, Amt and Freq contains only two options: ChemSTEER defaults from Table A-9 and User-defined. The conditional default and non-default options for Amt and Freq are presented in the tables below. Be sure to read the <u>ChemSTEER Estimation</u> <u>Methods and Models</u> topic for more information about changing model parameters.

You may not change the defining model parameter, LF, to be anything other than one of the defaults shown above. If you wish to model releases from drum residues using your own loss fraction, choose the <u>User-Defined Loss Rate Model</u>.

#### Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default characterizations for either Output 1 or Output 2 results are based on which LF is selected for the corresponding output:

- Results using the high end loss fractions (i.e., 0.03 for pumping or 0.006 for pouring) are characterized as *High End* by default.
- Results using the central tendency loss fractions (i.e., 0.025 for pumping or 0.003 for pouring) are characterized as *Central Tendency* by default.

You may select an alternative characterization for either of the outputs at any time.

#### **Default Model Basis**

The following default text is displayed in the Basis box on the View/Update Release Model Information screen:

"EPA/OPPT Drum Residual Model, CEB standard 3% residual"

Source/Activity Type/Operation Mode	Batch Condition	Operation Type	Conditional Amt Default (kg/site-day)	Non-default Options for Amt*
Container-Related / Continuous	Not Applicable	Any	For Ncd ≥ 1: MCi x Yi x Ncd (kg chemical/site-day) (from Container Parameters subtab of the Operation Parameters tab) For Ncd < 1: MCi x Yi (kg chemical/container) (from Container Parameters subtab of the	MCi (kg material/container) MCi x Yi (for Ncd ≥ 1 only) DMIchem DMOchem User-defined Amt
			Operation Parameters tab)	
Container-Related / Batch	Any	Any	For Ncd ≥ 1: MCi x Yi x Ncd (kg chemical/site-day) (from Container Parameters subtab of the Operation Parameters tab) For Ncd < 1: MCi x Yi (kg chemical/container) (from Container Parameters subtab of the Operation Parameters tab)	MCi (kg material/container) MCi x Yi (for Ncd ≥ 1 only) BMIchem BMOchem BMIchem x Ls (kg/site-bt) BMOchem x Ls (kg/site-bt) BMIchem x Nbd BMIchem x Nbd BMIchem x Nbd BMIchem x Nbd/Ls (kg/line-day) User-defined Amt
Not Container- Related / Continuous	Not Applicable	Manufacturing	DMOchem (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMIchem User-defined Amt
		Processing Use	DMIchem (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMOchem User-defined Amt
Not Container- Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of	Manufacturing	BMOchem (kg/line-bt) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMIchem x Ls (kg/site-bt) BMOchem x Ls (kg/site-bt)

# Table A-9a. Conditional Default Values for Amt for the EPA/OPPT Drum Residual Model

the Operation			User-defined Amt
Parameters tab)	Processing Use	BMIchem (kg/line-bt) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMIchem x Ls (kg/site-bt) BMOchem x Ls (kg/site-bt) User-defined Amt
Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Manufacturing	BMOchem x Nbd (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMOchem BMIchem x Nbd BMIchem x Nbd/Ls (kg/line-day) BMOchem x Nbd/Ls (kg/line-day) User-defined Amt
	Processing Use	BMIchem x Nbd (kg/site-day) (from the Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMOchem BMOchem x Nbd BMIchem x Nbd/Ls (kg/line-day) BMOchem x Nbd/Ls (kg/line-day) User-defined Amt

\*Non-default options for Amt are available by clicking in the *Type* column in the View/Update Release Model Information screen in the Releases tab.

Source/Activity Type/Operation Mode	Batch Condition	Conditional Freq Default (days of release/site-yr)	Non-Default Options for Freq*
Container- Related/Continuous	Not Applicable	For Ncd ≥ 1: ODa (from Container Parameters subtab of the Operation Parameters tab)	OD User-defined Freq
		For Ncd < 1: Ncy (containers/site-yr) (from Container Parameters subtab of the Operation Parameters tab)	
Container- Related/Batch	Any	For Ncd ≥ 1: ODa (from Container Parameters subtab of the Operation Parameters tab)	OD Nby User-defined Freq
		For Ncd < 1: Ncy (containers/site-yr) (from Container Parameters subtab of the Operation Parameters tab)	
Not Container- Related/Continuous	Not Applicable	OD (from Container Parameters subtab of the Operation Parameters tab)	User-defined Freq
Not Container- Related/Batch	Number of batches per day (Nbd)<1) (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby (from Container Parameters subtab of the Operation Parameters tab)	OD User-defined Freq
	Number of batches per day (Nbd)≥ 1) (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD (from Container Parameters subtab of the Operation Parameters tab)	Nby User-defined Freq

#### Table A-9b. Conditional Default Values for Freq for the EPA/OPPT Drum Residual Model

\*Non-default options for Freq are available by clicking in the *Type* column in the View/Update Release Model Information screen in the Releases tab.

## Key Rationale for Model

The three-percent loss is roughly equivalent to a one-inch heel in a standard 55-gallon drum. This is the basis for the high-end default estimate for pumping. Alternative, less conservative estimates obtained when liquids are poured from drums include 0.6% (high-end) and 0.3% (central tendency/mean).

#### References

US EPA Memo entitled Standard Assumptions for PMN Assessments from the Chemical Engineering Branch Quality Panel to Chemical Engineering Branch Staff and Management. 10/92.

PEI Associates for US EPA/OTS. Releases During Cleaning of Equipment. July 1988.

# EPA/OPPT Multiple Process Vessel Residual Model

#### **Model Description**

EPA assumes that 2% of the material being manufactured or processed remains as residual in the vessels after it is drained (via pump) following the operation.

#### Sources/Activities That Use This Model as a Default

The following sources/activities use the EPA/OPPT Multiple Process Vessel Residual Model as the default non-air release model:

• Equipment Cleaning Losses of Liquids from Multiple Vessels (see Equipment Cleaning Losses of Liquids)

#### **Other Sources/Activities**

The EPA/OPPT Multiple Process Vessel Residual Model may be an appropriate alternative to the default non-air release model for the following sources/activities:

• Equipment Cleaning Losses of Liquids from a Single, Small/Large Vessel (see Equipment Cleaning Losses of Liquids)

## Potential Media of Release

Water, Incineration, and/or Landfill (default: 100% of release to water)

#### Equations

For daily releases:

DR (kg/site-day) =  $LF \times Amt$ 

DR occurs over [Freq] days/year

For annual releases:

AR (kg/year) = DR × Freq × NS, AR is for all sites combined

## **Model Input Parameters and Default Values**

The EPA/OPPT Multiple Process Vessel Residual Model default values for each of the input parameters are summarized in Table A-10.

Parameter	Description	Default Value(s)	Units
LF	Loss fraction; fraction of an amount of the chemical that is estimated to be released	0.02 (conservative)	dimensionless
Amt	The amount of chemical to which a loss fraction is applied	Defaults specified in Table A-10a	kg/site-day
NS	Number of sites	NS (from Mass Balance Parameters subtab of Operation Parameters tab)	site(s)
Freq	The frequency of release of the chemical	Default specified in Table A-10b	day/site-year
DR	Daily Release rate	Calculated from model equation	kg/site-day
AR	Annual Release rate	Calculated from model equation	kg/year (all sites)

# Table A-10. Input Parameters and Default Values for the EPA/OPPT Multiple Process Vessel Residual Model

You may elect to change any parameter from Table A-10 except the model estimates DR and AR. Clicking the *Type* column for each changeable parameter other than LF, Amt and Freq contains only two options: ChemSTEER defaults from Table A-10 and User-defined. The conditional default and nondefault options for Amt and Freq are presented in the tables below. Be sure to read the <u>ChemSTEER</u> <u>Estimation Methods and Models</u> topic for more information about changing model parameters.

You may not change the defining model parameter, LF, to be anything other than one of the defaults shown above. If you wish to model releases from multiple process vessel residues using your own loss fraction, choose the <u>User-Defined Loss Rate Model</u>.

#### Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default Characterization of Output 1 Results: *Conservative* Default Characterization of Output 2 Results: *Conservative* 

You may select an alternative characterization for either of the outputs at any time.

## **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Release Model Information* screen:

"EPA/OPPT Multiple Process Vessel Residual Model, CEB standard 2% residual"

Source/Activity Type/Operation Mode	Batch Condition	Operation Type	Conditional Amt Default (kg/site-day)	Non-default Options for Amt*
Container-Related / Continuous	Not Applicable	Any	For Ncd ≥ 1: MCi x Yi x Ncd (kg chemical/site-day) (from Container Parameters subtab of the Operation Parameters tab) For Ncd < 1: MCi x Yi (kg chemical/container) (from Container Parameters subtab of the Operation Parameters tab)	MCi (kg material/container) MCi x Yi (for Ncd ≥ 1 only) DMIchem DMOchem User-defined Amt
Container-Related / Batch	Any	Any	For Ncd ≥ 1: MCi x Yi x Ncd (kg chemical/site-day) (from Container Parameters subtab of the Operation Parameters tab) For Ncd < 1: MCi x Yi (kg chemical/container) (from Container Parameters subtab of the Operation Parameters tab)	MCi (kg material/container) MCi x Yi (for Ncd ≥ 1 only) BMIchem BMOchem BMIchem x Ls (kg/site-bt) BMOchem x Ls (kg/site-bt) BMIchem x Nbd BMIchem x Nbd BMIchem x Nbd/Ls (kg/line-day) BMOchem x Nbd/Ls (kg/line-day) User-defined Amt
Not Container- Related / Continuous	Not Applicable	Manufacturing	DMOchem (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMIchem User-defined Amt
		Processing Use	DMIchem (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMOchem User-defined Amt
Not Container- Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance	Manufacturing	BMOchem (kg/line-bt) (from Mass Balance Parameters subtab of the Operation Parameters	BMIchem BMIchem x Ls (kg/site-bt) BMOchem x Ls

# Table A-10a. Conditional Default Values for Amt for the EPA/OPPT Multiple Process Vessel Residual Model

	Parameters subtab of the Operation Parameters tab)		tab)	(kg/site-bt) User-defined Amt
		Processing Use	BMIchem (kg/line-bt) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMIchem x Ls (kg/site-bt) BMOchem x Ls (kg/site-bt) User-defined Amt
	Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Manufacturing	BMOchem x Nbd (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMOchem BMIchem x Nbd BMIchem x Nbd/Ls (kg/line-day) BMOchem x Nbd/Ls (kg/line-day) User-defined Amt
		Processing Use	BMIchem x Nbd (kg/site-day) (from the Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMOchem BMOchem x Nbd BMIchem x Nbd/Ls (kg/line-day) BMOchem x Nbd/Ls (kg/line-day) User-defined Amt

\*Non-default options for Amt are available by clicking in the *Type* column in the View/Update Release Model Information screen in the Releases tab.

Source/Activity Type/Operation Mode	Batch Condition	Conditional Freq Default (days of release/site-yr)	Non-Default Options for Freq*
Container- Related/Continuous	Not Applicable	For Ncd ≥ 1: ODa (from Container Parameters subtab of the Operation Parameters tab)	OD User-defined Freq
		For Ncd < 1: Ncy (containers/site-yr) (from Container Parameters subtab of the Operation Parameters tab)	
Container- Related/Batch	Any	For Ncd ≥ 1: ODa (from Container Parameters subtab of the Operation Parameters tab)	OD Nby User-defined Freq
		For Ncd < 1: Ncy (containers/site-yr) (from Container Parameters subtab of the Operation Parameters tab)	
Not Container- Related/Continuous	Not Applicable	OD (from Container Parameters subtab of the Operation Parameters tab)	User-defined Freq
Not Container- Related/Batch	Number of batches per day (Nbd)<1) (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby (from Container Parameters subtab of the Operation Parameters tab)	OD User-defined Freq
	Number of batches per day (Nbd)≥ 1) (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD (from Container Parameters subtab of the Operation Parameters tab)	Nby User-defined Freq

# Table A-10b. Conditional Default Values for Freq for the EPA/OPPT Multiple Process Vessel Residual Model

\*Non-default options for Freq are available by clicking in the *Type* column in the View/Update Release Model Information screen in the Releases tab.

## Key Rationale for Model

Two percent of mass throughput based on the information and data in the July 1988 reference; the panel of chemical engineers with a variety of industrial experience considered this percentage to be a generally conservative estimate.

#### References

US EPA Memo entitled Standard Assumptions for PMN Assessments from the Chemical Engineering Branch Quality Panel to Chemical Engineering Branch Staff and Management. 10/92.

PEI Associates for US EPA/OTS. Releases During Cleaning of Equipment. July 1988.

# EPA/OPPT Single Vessel Residual Model

#### **Model Description**

EPA assumes that up to 1% of the material being manufactured or processed remains as residual in the vessel after it is drained (via pump) following the operation. Alternative assumptions include 0.2% high end and 0.07% central tendency for gravity-drained vessels.

#### Sources/Activities That Use This Model as a Default

The following sources/activities use the EPA/OPPT Single Process Vessel Residual Model as the default non-air release model:

- Equipment Cleaning Losses of Liquids from a Single, Small Vessel (see <u>Equipment</u> <u>Cleaning Losses of Liquids</u>)
- Equipment Cleaning Losses of Liquids from a Single, Large Vessel (see <u>Equipment</u> <u>Cleaning Losses of Liquids</u>)

#### **Other Sources/Activities**

The EPA/OPPT Single Process Vessel Residual Model may be an appropriate alternative to the default non-air release model for the following sources/activities:

• Equipment Cleaning Losses of Liquids from Multiple Vessels (see <u>Equipment Cleaning</u> Losses of Liquids)

#### **Potential Media of Release**

Water, Incineration, and/or Landfill (default: 100% of release to water)

#### Equations

For daily releases:

 $DR (kg/site-day) = LF \times Amt$ 

DR occurs over [Freq] days/year

For annual releases:

AR (kg/year) = DR × Freq × NS, AR is for all sites combined

#### Model Input Parameters and Default Values

The EPA/OPPT Single Process Vessel Residual Model default values for each of the input parameters are summarized in Table A-11.

Parameter	Description	Default Value(s)	Units
LF	Loss fraction; fraction of an amount of the chemical that is estimated to be released	Output 1:Default: 0.002 (High End to Bounding for gravity drain)Non-default option: 0.01 (Conservative); and 0.0007 (Central Tendency for gravity drain)Output 2:Default: 0.01 (Conservative for pumping) Non-default option: 0.002 (High End to Bounding ); and 0.0007 (Central Tendency for gravity drain)	dimensionless
Amt	The amount of chemical to which a loss fraction is applied	Defaults specified in Table A-11a	kg/site-day
NS	Number of sites	NS (from Mass Balance Parameters subtab of Operation Parameters tab)	site(s)
Freq	The frequency of release of the chemical	Default specified in Table A-11b	day/site-year
DR	Daily Release rate	Calculated from model equation	kg/site-day
AR	Annual Release rate	Calculated from model equation	kg/year (all sites)

 Table A-11. Input Parameters and Default Values for the EPA/OPPT Single Process Vessel Residual

 Model

You may elect to change any parameter from Table A-11 except the model estimates DR and AR. Clicking the *Type* column for each changeable parameter other than LF, Amt and Freq contains only two options: ChemSTEER defaults from Table A-11 and User-defined. The conditional default and nondefault options for Amt and Freq are presented in the tables below. Be sure to read the <u>ChemSTEER</u> <u>Estimation Methods and Models</u> topic for more information about changing model parameters.

You may not change the defining model parameter, LF, to be anything other than one of the defaults shown above. If you wish to model releases from a single process vessel residue using your own loss fraction, choose the <u>User-Defined Loss Rate Model</u>.

#### Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default characterizations for either Output 1 or Output 2 results are based on which LF is selected for the corresponding output:

• Results using the conservative loss fraction for pumping (i.e., 0.01) are characterized as *Conservative* by default.

- Results using the high end loss fraction for gravity draining (i.e., 0.002) are characterized as *High End to Bounding* by default.
- Results using the central tendency loss fraction for gravity draining (i.e., 0.0007) are characterized as *Central Tendency* by default.

You may select an alternative characterization for either of the outputs at any time.

#### **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Release Model Information* screen:

"EPA/OPPT Single Vessel Residual Model, CEB standard 1% residual"

Source/Activity Type/Operation Mode	Batch Condition	Operation Type	Conditional Amt Default (kg/site-day)	Non-default Options for Amt*
Container-Related / Continuous	Not Applicable	Any	For Ncd ≥ 1: MCi x Yi x Ncd (kg chemical/site-day) (from Container Parameters subtab of the Operation Parameters tab)	MCi (kg material/container) MCi x Yi (for Ncd ≥ 1 only) DMIchem DMOchem User-defined Amt
			For Ncd < 1: MCi x Yi (kg chemical/container) (from Container Parameters subtab of the Operation Parameters tab)	
Container-Related / Batch	Any	Any	For Ncd ≥ 1: MCi x Yi x Ncd (kg chemical/site-day) (from Container Parameters subtab of the Operation Parameters tab) For Ncd < 1: MCi x Yi (kg chemical/container) (from Container Parameters subtab of the Operation Parameters tab)	MCi (kg material/container) MCi x Yi (for Ncd ≥ 1 only) BMIchem BMOchem BMIchem x Ls (kg/site-bt) BMOchem x Ls (kg/site-bt) BMIchem x Nbd BMIchem x Nbd BMIchem x Nbd/Ls (kg/line-day) BMOchem x Nbd/Ls (kg/line-day) User-defined Amt
Not Container- Related / Continuous	Not Applicable	Manufacturing	DMOchem (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMIchem User-defined Amt
		Processing Use	DMIchem (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMOchem User-defined Amt
Not Container- Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance	Manufacturing	BMOchem (kg/line-bt) (from Mass Balance Parameters subtab of the Operation	BMIchem BMIchem x Ls (kg/site-bt) BMOchem x Ls

# Table A-11a. Conditional Default Values for Amt for the EPA/OPPT Single Process Vessel Residual Model

	Parameters subtab of the Operation Parameters tab)		Parameters tab)	(kg/site-bt)
				User-defined Amt
		Processing	BMIchem (kg/line-bt)	BMIchem
		Use	(from Mass Balance	BMIchem x Ls
			Parameters subtab of	(kg/site-bt)
			the Operation	BMOchem x Ls
			Parameters tab)	(kg/site-bt)
				User-defined Amt
	Number of batches	Manufacturing	BMOchem x Nbd	BMIchem
	per day		(kg/site-day)	BMOchem
	(Nbd) ≥ 1			BMIchem x Nbd
	(from Mass Balance		(from Mass Balance	BMIchem x Nbd/Ls
	Parameters subtab		Parameters subtab of	(kg/line-day)
	of the Operation		the Operation	BMOchem x Nbd/Ls
	Parameters tab)		Parameters tab)	(kg/line-day)
	·			User-defined Amt
		Processing	BMIchem x Nbd	BMIchem
		Use	(kg/site-day)	BMOchem
			(from the Mass Balance	BMOchem x Nbd
			Parameters subtab of	BMIchem x Nbd/Ls
			the Operation	(kg/line-day)
			Parameters tab)	BMOchem x Nbd/Ls
				(kg/line-day)
				User-defined Amt

\*Non-default options for Amt are available by clicking in the *Type* column in the View/Update Release Model Information screen in the Releases tab.
Source/Activity Type/Operation Mode	Batch Condition	Conditional Freq Default (days of release/site-yr)	Non-Default Options for Freq*
Container- Related/Continuous	Not Applicable	For Ncd ≥ 1: ODa (from Container Parameters subtab of the Operation Parameters tab)	OD User-defined Freq
		Ncy (containers/site-yr) (from Container Parameters subtab of the Operation Parameters tab)	
Container- Related/Batch	Any	For Ncd ≥ 1: ODa (from Container Parameters subtab of the Operation Parameters tab)	OD Nby User-defined Freq
		For Ncd < 1: Ncy (containers/site-yr) (from Container Parameters subtab of the Operation Parameters tab)	
Not Container- Related/Continuous	Not Applicable	OD (from Container Parameters subtab of the Operation Parameters tab)	User-defined Freq
Not Container- Related/Batch	Number of batches per day (Nbd)<1) (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby (from Container Parameters subtab of the Operation Parameters tab)	OD User-defined Freq
	Number of batches per day (Nbd)≥ 1) (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD (from Container Parameters subtab of the Operation Parameters tab)	Nby User-defined Freq

## Table A-11b. Conditional Default Values for Freq for the EPA/OPPT Single Process Vessel Residual Model

\*Non-default options for Freq are available by clicking in the *Type* column in the View/Update Release Model Information screen in the Releases tab.

## Key Rationale for Model

One percent of mass throughput based on the information and data (for pumping) in the July 1988 reference; the panel of chemical engineers with a variety of industrial experience considered this percentage to be a generally conservative estimate. Alternative, less conservative estimates obtained for gravity-drained vessels include 0.2% (high-end to bounding) and 0.07% (central tendency/mean).

## References

US EPA Memo entitled Standard Assumptions for PMN Assessments from the Chemical Engineering Branch Quality Panel to Chemical Engineering Branch Staff and Management. 10/92.

PEI Associates for US EPA/OTS. Releases During Cleaning of Equipment. July 1988.

## EPA/OPPT Small Container Residual Model

## **Model Description**

EPA assumes that liquids are poured from small shipping containers and that up to 0.6% (a central tendency of 0.3%) of the liquid originally in the container remains as residual after unloading.

## Sources/Activities That Use This Model as a Default

The following sources/activities use the EPA/OPPT Small Container Residual Model as the default for calculating non-releases:

- Cleaning Liquid Residuals from Bottles Used to Transport the Raw Material/Product (see <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>)
- Cleaning Liquid Residuals from Small Containers Used to Transport the Raw Material/Product (see <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>)

## **Other Sources/Activities**

The EPA/OPPT Small Container Residual Model may be an appropriate alternative to the default non-air release model for the following sources/activities:

- Cleaning Liquid Residuals from Containers Used to Transport the Raw Material/Product (see <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>)
- Cleaning Liquid Residuals from Storage/Transport Vessels (User-defined) (see <u>Cleaning</u> <u>Liquid Residuals from Transport Containers/Vessels</u>)

## **Potential Media of Release**

Water, Incineration, and/or Landfill (default: 100% of release to water)

NOTE: a 1994 policy decision was issued to account for uncertainties in media of releases, and many residual releases are assumed to be released to water as a default. This 1994 decision supersedes the default medium of release that is listed in the 1992 reference memorandum.

## Equations

For daily releases:

DR (kg/site-day) = LF × Amt DR occurs over [Freq] days/year For annual releases:

AR (kg/year) = DR × Freq × NS, AR is for all sites combined

## Model Input Parameters and Default Values

The EPA/OPPT Small Container Residual Model default values for each of the input parameters are summarized in Table A-12.

Table A 12 In	nut Paramotors an	d Dofault Values	for the EDA /		ontainar E	Posidual Ma	امه
Table A-12. In	put Parameters and	u Delault values	ior the EPA/	UPPT Small C	опташег в	lesidual ivio	uer

Parameter	Description	Default Value(s)	Units
LF	Loss fraction; fraction of an amount of the chemical that is estimated to be released	Output 1: <u>Default:</u> 0.003 (Central Tendency) <u>Non-default option:</u> 0.006 (High End)	dimensionless
		<i>Output 2:</i> <u>Default:</u> 0.006 (High End) <u>Non-default option:</u> 0.003 (Central Tendency)	
Amt	The amount of chemical to which a loss fraction is applied	Defaults specified in Table A-12a	kg/site-day
NS	Number of sites	NS (from Mass Balance Parameters subtab of Operation Parameters tab)	site(s)
Freq	The frequency of release of the chemical	Default specified in Table A-12b	day/site-year
DR	Daily Release rate	Calculated from model equation	kg/site-day
AR	Annual Release rate	Calculated from model equation	kg/year (all sites)

You may elect to change any parameter from Table A-12 except the model estimates DR and AR. Clicking the *Type* column for each changeable parameter other than LF, Amt and Freq contains only two options: ChemSTEER defaults from Table A-12 and User-defined. The conditional default and nondefault options for Amt and Freq are presented in the tables below. Be sure to read the <u>ChemSTEER</u> <u>Estimation Methods and Models</u> topic for more information about changing model parameters.

You may not change the defining model parameter, LF, to be anything other than one of the defaults shown above. If you wish to model releases from small container residues using your own loss fraction, choose the <u>User-Defined Loss Rate Model</u>.

## Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default characterizations for either Output 1 or Output 2 results are based on which LF is selected for the corresponding output:

• Results using the high end loss fraction (i.e., 0.006) are characterized as *High End* by default.

• Results using the central tendency loss fraction (i.e., 0.003) are characterized as *Central Tendency* by default.

You may select an alternative characterization for either of the outputs at any time.

## **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Release Model Information* screen:

"EPA/OPPT Small Container Residual Model, CEB standard 0.6% residual"

Source/Activity Type/Operation Mode	Batch Condition	Operation Type	Conditional Amt Default (kg/site-day)	Non-default Options for Amt*
Container-Related / Continuous	Not Applicable	Any	For Ncd ≥ 1: MCi x Yi x Ncd (kg chemical/site-day) (from Container Parameters subtab of the Operation Parameters tab) For Ncd < 1: MCi x Yi (kg chemical/container) (from Container	MCi (kg material/container) MCi x Yi (for Ncd ≥ 1 only) DMIchem DMOchem User-defined Amt
			Parameters subtab of the Operation Parameters tab)	
Container-Related / Batch	Any	Any	For Ncd ≥ 1: MCi x Yi x Ncd (kg chemical/site-day) (from Container Parameters subtab of the Operation Parameters tab) For Ncd < 1: MCi x Yi (kg chemical/container) (from Container Parameters subtab of the Operation Parameters tab)	MCi (kg material/container) MCi x Yi (for Ncd ≥ 1 only) BMIchem BMOchem BMIchem x Ls (kg/site-bt) BMOchem x Ls (kg/site-bt) BMIchem x Nbd BMIchem x Nbd BMIchem x Nbd/Ls (kg/line-day) BMOchem x Nbd/Ls (kg/line-day) User-defined Amt
Not Container- Related / Continuous	Not Applicable	Manufacturing	DMOchem (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMIchem User-defined Amt
		Processing Use	DMIchem (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMOchem User-defined Amt
Not Container- Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab	Manufacturing	BMOchem (kg/line-bt) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMIchem x Ls (kg/site-bt) BMOchem x Ls (kg/site-bt)

## Table A-12a. Conditional Default Values for Amt for the EPA/OPPT Small Container Residual Model

of the Operation			User-defined Amt
Parameters tab)	Processing Use	BMIchem (kg/line-bt) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMIchem x Ls (kg/site-bt) BMOchem x Ls (kg/site-bt) User-defined Amt
Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Manufacturing	BMOchem x Nbd (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMOchem BMIchem x Nbd BMIchem x Nbd/Ls (kg/line-day) BMOchem x Nbd/Ls (kg/line-day) User-defined Amt
	Processing Use	BMIchem x Nbd (kg/site-day) (from the Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMOchem BMOchem x Nbd BMIchem x Nbd/Ls (kg/line-day) BMOchem x Nbd/Ls (kg/line-day) User-defined Amt

\*Non-default options for Amt are available by clicking in the Type column in the View/Update Release Model Information screen in the Releases tab.

Source/Activity Type/Operation Mode	Batch Condition	Conditional Freq Default (days of release/site-yr)	Non-Default Options for Freq*
Container- Related/Continuous	Not Applicable	For Ncd ≥ 1: ODa (from Container Parameters subtab of the Operation Parameters tab)	OD User-defined Freq
		For Ncd < 1: Ncy (containers/site-yr) (from Container Parameters subtab of the Operation Parameters tab)	
Container- Related/Batch	Any	For Ncd ≥ 1: ODa (from Container Parameters subtab of the Operation Parameters tab)	OD Nby User-defined Freq
		For Ncd < 1: Ncy (containers/site-yr) (from Container Parameters subtab of the Operation Parameters tab)	
Not Container- Related/Continuous	Not Applicable	OD (from Container Parameters subtab of the Operation Parameters tab)	User-defined Freq
Not Container- Related/Batch	Number of batches per day (Nbd)<1) (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby (from Container Parameters subtab of the Operation Parameters tab)	OD User-defined Freq
	Number of batches per day (Nbd)≥ 1) (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD (from Container Parameters subtab of the Operation Parameters tab)	Nby User-defined Freq

## Table A-12b. Conditional Default Values for Freq for the EPA/OPPT Small Container Residual Model

\*Non-default options for Freq are available by clicking in the *Type* column in the View/Update Release Model Information screen in the Releases tab.

## Key Rationale for Model

The six tenths and three tenths of one percent loss are high end and central tendency values, respectively, in a range of values from an EPA sponsored study residuals in containers from which liquids have been poured.

## References

US EPA Memo entitled Standard Assumptions for PMN Assessments from the Chemical Engineering Branch Quality Panel to Chemical Engineering Branch Staff and Management. 10/92.

PEI Associates for US EPA/OTS. Releases During Cleaning of Equipment. July 1988.

## EPA/OPPT Solid Residuals in Transport Containers Model

## **Model Description**

EPA assumes that solids are transferred from shipping containers and that up to 1% (by weight) of the solids originally in the container remains as residual after unloading.

## Sources/Activities That Use This Model as a Default

The following sources/activities use the EPA/OPPT Solid Residuals in Transport Containers Model as the default for calculating non-air releases:

- All sources/activities for <u>Cleaning Solid Residuals from Transport Containers/Vessels</u>
- Equipment Cleaning Losses of Solids from Process Vessels

This model is not used as an alternative release model for any other sources/activities.

## **Potential Media of Release**

Water, Incineration, and/or Landfill (default: 100% of release to water)

## Equations

For daily releases:

DR (kg/site-day) = LF × Amt

DR occurs over [Freq] days/year

For annual releases:

AR (kg/year) = DR × Freq × NS, AR is for all sites combined

## **Model Input Parameters and Default Values**

The EPA/OPPT Solid Residual in Transport Containers Model default values for each of the input parameters are summarized in Table A-13.

Parameter	Description	Default Value(s)	Units
LF	Loss fraction; fraction of an amount of the chemical that is estimated to be released	0.01 (not characterized)	dimensionless
Amt	The amount of chemical to which a loss fraction is applied	Defaults specified in Table A-13a	kg/site-day
NS	Number of sites	NS (from Mass Balance Parameters subtab of Operation Parameters tab)	site(s)
Freq	The frequency of release of the chemical	Default specified in Table A-13b	day/site-year
DR	Daily Release rate	Calculated from model equation	kg/site-day
AR	Annual Release rate	Calculated from model equation	kg/year (all sites)

# Table A-13. Input Parameters and Default Values for the EPA/OPPT Solid Residuals in Transport Containers Model

You may elect to change any parameter from Table A-13 except the model estimates DR and AR. Clicking the *Type* column for each changeable parameter other than LF, Amt and Freq contains only two options: ChemSTEER defaults from Table A-13 and User-defined. The conditional default and non-default options for Amt and Freq are presented in the tables below. Be sure to read the <u>ChemSTEER</u> <u>Estimation Methods and Models</u> topic for more information about changing model parameters.

You may not change the defining model parameter, LF, to be anything other than one of the defaults shown above. If you wish to model releases of container solid residues using your own loss fraction, choose the <u>User-Defined Loss Rate Model</u>.

## Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default Characterization of Output 1 Results: *Output 1* Default Characterization of Output 2 Results: *Output 2* 

You may select an alternative characterization for either of the outputs at any time.

Default Model Basis

The following default text is displayed in the *Basis* box on the *View/Update Release Model Information* screen:

"EPA/OPPT Solid Residuals in Transport Containers Model, CEB standard 1% residual"

Source/Activity Type/Operation Mode	Batch Condition	Operation Type	Conditional Amt Default (kg/site-day)	Non-default Options for Amt*
Container-Related / Continuous	Not Applicable	Any	For Ncd ≥ 1: MCi x Yi x Ncd (kg chemical/site-day) (from Container Parameters subtab of the Operation Parameters tab)	MCi (kg material/container) MCi x Yi (for Ncd ≥ 1 only) DMIchem DMOchem User-defined Amt
			For Ncd < 1: MCi x Yi (kg chemical/container) (from Container Parameters subtab of the Operation Parameters tab)	
Container-Related / Batch	Any	Any	For Ncd ≥ 1: MCi x Yi x Ncd (kg chemical/site-day) (from Container Parameters subtab of the Operation Parameters tab) For Ncd < 1:	MCi (kg material/container) MCi x Yi (for Ncd ≥ 1 only) BMIchem BMOchem BMIchem x Ls (kg/site-bt)
			MCi x Yi (kg chemical/container) (from Container Parameters subtab of the Operation Parameters tab)	BMOchem x Ls (kg/site-bt) BMIchem x Nbd BMOchem x Nbd/Ls (kg/line-day) BMOchem x Nbd/Ls (kg/line-day) User-defined Amt
Not Container- Related / Continuous	Not Applicable	Manufacturing	DMOchem (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMIchem User-defined Amt
		Processing Use	DMIchem (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMOchem User-defined Amt
Not Container- Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance	Manufacturing	BMOchem (kg/line-bt) (from Mass Balance Parameters subtab of the Operation	BMIchem BMIchem x Ls (kg/site-bt) BMOchem x Ls

# Table A-13a. Conditional Default Values for Amt for the EPA/OPPT Solid Residuals in Transport Containers Model

	Parameters subtab of the Operation Parameters tab)		Parameters tab)	(kg/site-bt) User-defined Amt
		Processing Use	BMIchem (kg/line-bt) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMIchem x Ls (kg/site-bt) BMOchem x Ls (kg/site-bt) User-defined Amt
	Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Manufacturing	BMOchem x Nbd (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMOchem BMIchem x Nbd BMIchem x Nbd/Ls (kg/line-day) BMOchem x Nbd/Ls (kg/line-day) User-defined Amt
		Processing Use	BMIchem x Nbd (kg/site-day) (from the Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMOchem BMOchem x Nbd BMIchem x Nbd/Ls (kg/line-day) BMOchem x Nbd/Ls (kg/line-day) User-defined Amt

\*Non-default options for Amt are available by clicking in the Type column in the View/Update Release Model Information screen in the Releases tab.

Source/Activity Type/Operation Mode	Batch Condition	Conditional Freq Default (days of release/site-yr)	Non-Default Options for Freq*
Container- Related/Continuous	Not Applicable	For Ncd ≥ 1: ODa (from Container Parameters subtab of the Operation Parameters tab)	OD User-defined Freq
		For Ncd < 1: Ncy (containers/site-yr) (from Container Parameters subtab of the Operation Parameters tab)	
Container- Related/Batch	Any	For Ncd ≥ 1: ODa (from Container Parameters subtab of the Operation Parameters tab)	OD Nby User-defined Freq
		For Ncd < 1: Ncy (containers/site-yr) (from Container Parameters subtab of the Operation Parameters tab)	
Not Container- Related/Continuous	Not Applicable	OD (from Container Parameters subtab of the Operation Parameters tab)	User-defined Freq
Not Container- Related/Batch	Number of batches per day (Nbd)<1) (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby (from Container Parameters subtab of the Operation Parameters tab)	OD User-defined Freq
	Number of batches per day (Nbd)≥ 1) (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD (from Container Parameters subtab of the Operation Parameters tab)	Nby User-defined Freq

# Table A-13b. Conditional Default Values for Freq for the EPA/OPPT Solid Residuals in TransportContainers Model

\*Non-default options for Freq are available by clicking in the *Type* column in the View/Update Release Model Information screen in the Releases tab.

## Key Rationale for Model

The one percent loss is a value based on an extrapolation of a range of values from an EPA sponsored study of residuals in containers from which liquids have been poured

## References

US EPA Memo entitled Standard Assumptions for PMN Assessments from the Chemical Engineering Branch Quality Panel to Chemical Engineering Branch Staff and Management. 10/92.

PEI Associates for US EPA/OTS. Releases During Cleaning of Equipment. July 1988.

## EPA/OPPT Water Saturation Loss Model

#### **Model Description**

EPA assumes that water contacted with a mass of material containing the chemical becomes saturated with the chemical. This water saturated with the chemical is wasted or disposed.

## Sources/Activities That Use This Model as a Default

The following sources/activities use EPA/OPPT Water Saturation Loss Model as the default for calculating non-air releases:

<u>Aqueous Wash of Organic Mass</u>

## **EPA/OPPT** Water Saturation Loss Model – Other Sources/Activities

The EPA/OPPT Water Saturation Loss Model may be an appropriate alternative to the default non-air release model for the following sources/activities:

• <u>Miscellaneous Sources/Activities</u>.

#### **Potential Media of Release**

Water, Incineration, and/ or Landfill (default: 100% of release to water)

## Equations

For daily releases:

DR (kg/site-day) = WSchem × CF × Amt / 1000

DR occurs over [Freq] days/year

For annual releases:

AR (kg/year) = DR × Freq × NS, AR is for all sites combined

## **Model Input Parameters and Default Values**

The EPA/OPPT Water Saturation Loss Model default values for each of the input parameters are summarized in Table A-14.

Parameter	Description	Default Value(s)	Units
WSchem	Water solubility of the chemical	WSchem (from chemical tab)	g/L
CF	Correction factor*	1	dimensionless
Amt	An amount of water in which the chemical reaches saturation	Value based on Table A-14a	kg/site-day
NS	Number of sites	NS (from Mass Balance Parameters subtab of Operation Parameters tab)	site(s)
Freq	The frequency of release of the chemical	Default specified in Table A-14b	day/site-year
DR	Daily Release rate	Calculated from model equation	kg/site-day
AR	Annual Release rate	Calculated from model equation	kg/year (all sites)

## Table A-14. Input Parameters and Default Values for the EPA/OPPT Water Saturation Loss Model

\*A factor that you may adjust to account for: (1) multiples of an amount (Amt) of water (e.g., multiple washings); (2) a known or estimated correction of the water solubility of the chemical; and/ or (3) other corrections.

You may elect to change any parameter from Table A-14 except the model estimates DR and AR. Clicking the *Type* column for each changeable parameter other than Amt and Freq contains only two options: ChemSTEER defaults from Table A-14 and User-defined. The conditional default and nondefault options for Amt and Freq are presented in the tables below. Be sure to read the <u>ChemSTEER</u> <u>Estimation Methods and Models</u> topic for more information about changing model parameters.

## Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default Characterization of Output 1 Results: *Output 1* Default Characterization of Output 2 Results: *Output 2* 

You may select an alternative characterization for either of the outputs at any time.

## **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Release Model Information* screen:

"EPA/OPPT Water Saturation Loss Model"

Source/Activity Type/Operation Mode	Batch Condition	Operation Type	Conditional Amt Default (kg/site-day)	Non-default Options for Amt*
Container-Related / Continuous	Not Applicable	Any	For Ncd ≥ 1: MCi x Ncd (kg material/site-day) (from Container Parameters subtab of the Operation Parameters tab) For Ncd < 1:	MCi (for Ncd ≥ 1 only) DMIrm DMOprod User-defined Amt
			MCi (kg material/container) (from Container Parameters subtab of the Operation Parameters tab)	
Container-Related / Batch	Any	Any	For Ncd ≥ 1: MCi x Ncd (kg material/site-day) (from Container Parameters subtab of the Operation Parameters tab)	MCi (for Ncd ≥ 1 only) BMIrm BMOprod BMIrmx Ls (kg/site- bt) BMOprod x Ls
			For Ncd < 1: MCi (kg material/container) (from Container Parameters subtab of the Operation Parameters tab)	(kg/site-bt) BMIrm x Nbd BMOprod x Nbd BMIrm x Nbd/Ls (kg/line-day) BMOprod x Nbd/Ls (kg/line-day) User-defined Amt
Not Container- Related / Continuous	Not Applicable	Manufacturing	DMOprod (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMIrm User-defined Amt
		Processing Use	DMIrm (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMOprod User-defined Amt
Not Container- Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation	Manufacturing	BMOprod (kg/line-bt) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIrm BMIrm x Ls (kg/site- bt) BMOprod x Ls (kg/site-bt) User-defined Amt
	Parameters tab)	Processing	BMIrm (kg/line-bt)	BMIrm

## Table A-14a. Conditional Default Values for Amt for the EPA/OPPT Water Saturation Loss Model

	Use	(from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIrm x Ls (kg/site- bt) BMOprod x Ls (kg/site-bt) User-defined Amt
Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Manufacturing	BMOprod x Nbd (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIrm BMOprod BMIrm x Nbd BMIrm x Nbd/Ls (kg/line-day) BMOprod x Nbd/Ls (kg/line-day) User-defined Amt
	Processing Use	BMIrm x Nbd (kg/site-day) (from the Mass Balance Parameters subtab of the Operation Parameters tab)	BMIrm BMOprod BMOprod x Nbd BMIrm x Nbd/Ls (kg/line-day) BMOprod x Nbd/Ls (kg/line-day) User-defined Amt

\*Amt (of water) defaults correspond to throughput volumes of materials processed (e.g., if 10,000 kg/day of product is produced in the operation, the default Amt (amount of water) contacting the batch of material containing the chemical is also 10,000 kg/day).

\*\*Non-default options for Amt are available by clicking in the Type column in the View/Update Release Model Information screen in the Releases tab.

Source/Activity Type/Operation Mode	Batch Condition	Conditional Freq Default (days of release/site-yr)	Non-Default Options for Freq*
Container- Related/Continuous	Not Applicable	For Ncd ≥ 1: ODa (from Container Parameters subtab of the Operation Parameters tab)	OD User-defined Freq
		For Ncd < 1: Ncy (containers/site-yr) (from Container Parameters subtab of the Operation Parameters tab)	
Container- Related/Batch	Any	For Ncd ≥ 1: ODa (from Container Parameters subtab of the Operation Parameters tab)	OD Nby User-defined Freq
		For Ncd < 1: Ncy (containers/site-yr) (from Container Parameters subtab of the Operation Parameters tab)	
Not Container- Related/Continuous	Not Applicable	OD (from Container Parameters subtab of the Operation Parameters tab)	User-defined Freq
Not Container- Related/Batch	Number of batches per day (Nbd)<1) (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby (from Container Parameters subtab of the Operation Parameters tab)	OD User-defined Freq
	Number of batches per day (Nbd)≥ 1) (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD (from Container Parameters subtab of the Operation Parameters tab)	Nby User-defined Freq

## Table A-14b. Conditional Default Values for Freq for the EPA/OPPT Water Saturation Loss Model

\*Non-default options for Freq are available by clicking in the *Type* column in the View/Update Release Model Information screen in the Releases tab.

## Key Rationale for Model

Water contacted with a mass of material containing the chemical can become partially or fully saturated with the chemical as the chemical dissolves in the water, or chemical can be entrained in the water at levels below or above the saturation level. Assuming water saturation allows for a rough estimation when not enough information is available to make other estimates.

## Reference

## NA

## EPA/OPPT Cooling Tower Blowdown Loss Model

## **Model Description**

This model estimates releases of a cooling tower additive chemical as a result of periodic blowdown of the recirculating fluid (e.g., water). This model assumes that 0.6 percent of the cooling tower's recirculation rate is discharged during blowdown.

NOTE: This model is a default model for estimating releases to water from the <u>Recirculating</u> <u>Water-Cooling Tower Additive Releases</u> source/activity. This model may not be used for any other source/activity in ChemSTEER.

## **Potential Media of Release**

Air, Incineration, Landfill and/or Water (default: 100% release to water)

## Equations

For daily releases:

DR (kg/site-day) = LF × Amt

DR occurs over [Freq] days/year

For annual releases:

AR (kg/year) = DR × Freq × NS, AR is for all sites combined

## **Model Input Parameters and Default Values**

The EPA/OPPT Cooling Tower Blowdown Loss Model default values for each of the input parameters are summarized in Table A-15.

Parameter	Description	Default Value(s)	Units
LF	Loss fraction; fraction of an amount of the chemical that is estimated to be released	Value of LFb from Mass Balance subtab <i>Daily</i> <i>Mass of Chemical Used (DMUchem)</i> screen; ChemSTEER default for LFb is 0.006	dimensionless
Amt	The amount of chemical to which a loss fraction is applied	Value of DRR chem from Mass Balance subtab Daily Mass of Chemical Used (DMUchem) screen	kg/site-day
Freq	The frequency of release of the chemical	OD (from Mass Balance Parameters subtab of Operation Parameters tab)	days/site-year
NS	Number of sites	NS (from Mass Balance Parameters subtab of Operation Parameters tab)	site(s)
DR	Total daily release rate of tower blowdown	Calculated from model equation	kg/site-day
AR	Total annual release rate of tower blowdown	Calculated from model equation	kg/year (all sites)

## Table A-15. Input Parameters and Default Values for the EPA/OPPT Cooling Tower Blowdown Loss Model

You may not change any parameter from Table A-15.

#### Default Parameter Value Switch Settings and Results Characterization:

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default characterizations for either Output 1 or Output 2 results are What-if.

You may select an alternative characterization for either of the outputs at any time.

## **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Release Model Information* screen:

"EPA/OPPT Cooling Tower Blowdown Loss Model; up to 0.6% of the tower recirculation rate"

#### Key Rationale for Model

To control the unwanted accumulation of nonvolatile components in a water-cooling tower, periodic blowdown of the recirculating water must be performed. This model assumes as a default that 0.6% of the tower's recirculation rate is released to on- and/or off-site wastewater treatment as a result of blowdown.

## Reference

Summary Sheet: Recirculating Water-Cooling Tower, No date.

## EPA/OPPT Solids Transfer Dust Loss Model

## **Model Description**

This model estimates the environmental release of solids during transfer activities (i.e., unloading and loading), and includes options for apportioning the release to various receiving media based on the type of control technology employed.

## Sources/Activities That Use This Model as a Default

The following sources/activities use the EPA/OPPT Solids Transfer Dust Loss Model as the default for calculating releases of a chemical to air, water, incineration, or landfill:

- Unloading Solids from Transport Containers/Vessels (Raw Material or Product)
- Loading Solids into Transport Containers/Vessels (Raw Material or Product)

This model applies to loading/unloading of solid raw materials or products. It does not apply to solid equipment cleaning, filter media changeout, or any other activities that may generate a dust (e.g., milling).

## **Potential Media of Release**

The potential media of release and fraction of the total release to each are dependent upon the optional dust emission control technology that is selected. These options are summarized in Table A-16c.

**NOTE:** If you change the value(s) of DstCntrl and/or SrE and click *OK* in the *View / Update Release model Information* screen, the values of the percent to each medium of release will be automatically updated according to the equations in Table A-16c. If you had previously changed the media of release designations to non-default percentages, the changes will be overwritten, and you will need to return to the Modify Media of Release window to re-enter your changes.

## Equations

For daily releases:

DR (kg/site-day) = LF x Amt

DR occurs over [Freq] days/year

For annual releases:

AR (kg/year) = DR x Freq x NS, AR is for all sites combined

## Model Input Parameters and Default Values

The EPA/OPPT Solids Transfer Dust Loss Model default values for each of the input parameters are summarized in Table A-16.

Parameter	Description	Default Value(s)	Units
LF	Loss fraction; fraction of an amount of the chemical that is estimated to be released	0.005 (conservative)	dimensionless
Amt	The amount of chemical to which a loss fraction is applied	Defaults specified in Table A-16a	kg/site-day
NS	Number of sites	NS (from Mass Balance Parameters subtab of Operation Parameters tab)	site(s)
Freq	The frequency of release of the chemical	Defaults specified in Table A-16b	days/site-year
DstCntrl	Dust control technology	<ul> <li><u>Default:</u> 0 (None)</li> <li>Non-default options (see Table A-16c):</li> <li>Fabric filter/baghouse</li> <li>Mechanical/cyclone collectors</li> </ul>	NA
SrE*	Solid removal efficiency of dust control technology	Defaults specified in Table A-16c	dimensionless
DR	Daily release rate	Calculated from model equation	kg/site-day
AR	Annual release rate	Calculated from model equation	kg/year (all sites)

## Table A-16. Input Parameters and Default Values for the EPA/OPPT Solids Transfer Dust Loss Model

\*SrE is not used in the release calculations. It is used to specify the default media of release designations and/or percentages Update Release Media Output Specification screen of the Releases tab.

You may elect to change any parameter from Table A-16 except the model estimates DR and AR. Clicking the *Type* column for each changeable parameter other than LF, Amt and Freq contains only two options: ChemSTEER defaults from Table A-16 and User-defined. The conditional default and non-default options for Amt, Freq, and SrE are presented in the tables below. Be sure to read the <u>ChemSTEER Estimation Methods and Models</u> topic for more information about changing model parameters.

You may not change the defining model parameter, LF, to be anything other than the default shown above. If you wish to model dust releases from solids transfer activities using your own loss fraction, choose the <u>User-Defined Loss Rate Model</u>.

## Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default Characterization of Output 1 Results: *Conservative* Default Characterization of Output 2 Results: *Conservative* 

You may select an alternative characterization for either of the outputs at any time.

## Default Model Basis

The following default text is displayed in the *Basis* box on the *View/Update Release Model Information* screen:

"EPA/OPPT Solids Transfer Dust Loss Model"

If DstCntrl is None, then add, "No dust controls are assumed as a worst case"

Otherwise add, "Dust emissions controlled by" [DstCntrl]

\*It is recommended that you update this default text as appropriate, especially to specify a user-defined control technology.

## Table A-16a. Conditional Default Values for Amt for the EPA/OPPT Solids Transfer Dust Loss Model

Source/Activity Type/Operation Mode	Batch Condition	Operation Type	Conditional Amt Default (kg/site-day)	Non-default Options for Amt*
Container-Related / Continuous	Not Applicable	Any	MCi x Yi x Ncd (kg chemical/site-day) (from Container Parameters subtab of the Operation Parameters tab)	MCi (kg material/container) MCi x Yi (for Ncd ≥ 1 only) DMIchem DMOchem User-defined Amt
Container-Related / Batch	Any	Any	MCi x Yi x Ncd (kg chemical/site-day) (from Container Parameters subtab of the Operation Parameters tab)	MCi (kg material/container) MCi x Yi (for Ncd ≥ 1 only) BMIchem BMOchem BMIchem x Ls (kg/site-bt) BMOchem x Ls (kg/site-bt) BMIchem x Nbd BMOchem x Nbd BMIchem x Nbd/Ls (kg/line- day) BMOchem x Nbd/Ls (kg/line-day) User-defined Amt

\*Non-default options for Amt are available by clicking in the *Type* column in the View/Update Release Model Information screen in the Releases tab.

Source/Activity Type/Operation Mode	Batch Condition	Conditional Freq Default (days of release/site-yr)	Non-Default Options for Freq*
Container- Related/Continuous	Not Applicable	ODa (from Container Parameters subtab of the Operation Parameters tab)	OD User-defined Freq
Container- Related/Batch	Any	ODa (from Container Parameters subtab of the Operation Parameters tab)	OD Nby User-defined Freq

## Table A-16b. Conditional Default Values for Freq for the EPA/OPPT Solids Transfer Dust Loss Model

\*Non-default options for Freq are available by clicking in the *Type* column in the View/Update Release Model Information screen in the Releases tab.

# Table A-16c. Conditional Default Values for Solids Removal Efficiency and Media of Release for the EPA/OPPT Solids Transfer Dust Loss Model

Dust Control Technology Setting (DstCntrl) <sup>1</sup>	Solids Removal Efficiency (SrE) (dimensionless)	Default Media of Release Designations <sup>2</sup> (in the Update Release Media Output Specification screen of the Releases tab)
None (default)	0	% to Water or Air or Incineration or Landfill = 100
Mechanical collector/cyclone	<u>Non-default option<sup>4</sup></u> : 0.8 (low end; conservative) <u>Non-default option<sup>3,4</sup></u> : 0.99 (high end)	% to Incineration or Landfill = SrE x 100 % to Water or Air or Landfill = (1-SrE) x 100
Fabric filter/baghouse	<u>Non-default option<sup>4</sup></u> : 0.99 (conservative)	% to Incineration or Landfill = SrE x 100 % to Water or Air or Landfill = (1-SrE) x 100

1. The model also indicates that scrubber control technology efficiency varies. Consult Figure 7-1 of the CEB Engineering Manual (EPA 1991).

2. You may modify the default media of release designations and/or percentages directly in the Update Release Media Output Specification screen of the Releases tab.

3. Non-default options for SrE are available by clicking in the *Type* column in the View/Update Release Model Information screen in the Releases tab.

4. EPA 1991

## Key Rationale for Model

The 0.5-percent loss rate (EPA, 2006) is the median of the upper bounds of dust loss data found in available sources. Default solids removal efficiencies for each of the control technology options are based on standard CEB low end/conservative estimates (EPA 1991).

## References

US EPA Chemical Engineering Branch model entitled, Generic Model to Estimate Dust Releases from Transfer/Unloading Operations of Solid Powders; July 20, 2007.

Chapter 7 of the Chemical Engineering Branch Manual for the Preparation of Engineering Assessments; Washington, DC; Office of Toxic Substances, U.S. Environmental Protection Agency; 1991; pp. 7-3 through 7-9.

Models for Calculating Multi-Media Releases

## EPA/OPPT Automobile OEM Coating Overspray Loss Model

## **Model Description**

This model estimates releases of overspray of *non-volatile* chemical in coatings during their application to OEM automobiles using spray guns within a spray booth with controls to capture overspray.

#### Sources/Activities That Use This Model as a Default

The EPA/OPPT Automobile OEM Coating Overspray Loss Model is the default for calculating multi-media releases of a chemical to air, as well as water, incineration, or landfill for the <u>Automobile</u> <u>OEM Spray Coating Application</u> source/activity.

This model is not used as an alternative release model for any other sources/activities.

#### **Potential Media of Release**

Air, Incineration, Landfill and/or Water (see Default Media of Release section below)

## **Default Media of Release**

% to Air = (1-McE) × 100 % to Water = McE × (1- SrE) × 100 % to Landfill = McE × SrE × 100

**NOTE:** If you change the value(s) of McE and/or SrE and click *OK* in the *View / Update Release Model Information* screen, the values of the percent to each medium of release will be automatically updated according to the above equations. If you had previously changed the media of release designations to non-default percentages, the changes will be overwritten, and you will need to return to the Modify Media of Release window to re-enter your changes.

#### Equations

For daily releases: DR (kg/site-day) = LF x Amt DR occurs over [Freq] days/year

For annual releases: AR (kg/year) = DR x Freq x NS, AR is for all sites combined

## **Model Input Parameters and Default Values**

The EPA/OPPT Automobile OEM Coating Overspray Loss Model (non-volatiles) default values for each of the input parameters are summarized in Table A-17.

Table A-17. Input Parameters and Default Values for the EPA/OPPT Automobile OEM Coating
Overspray Loss Model (non-volatiles)

Parameter	Description	Default Value(s)	Units
LF	Loss fraction; fraction of an amount of the chemical that is estimated to be released	1-TE	dimensionless
TE	Spray gun transfer efficiency	Value based on Table A-17a	dimensionless
McE	Spray mist capture efficiency	Output 1: <u>Default:</u> 0.96 (waterwash/dry filter default) <u>Non-default options:</u> User-defined McE Output 2: <u>Default:</u> 0.96 (waterwash/dry filter default)	dimensionless
SrE	Solid removal efficiency from captured mist	Output 1: <u>Default:</u> 1 (dry filter default) <u>Non-default option:</u> 0.90 (waterwash); and User-defined SrE	dimensionless
		Output 2: <u>Default:</u> 0.90 (waterwash default) <u>Non-default option:</u> 1 (dry filter); and User-defined SrE	
Amt	The amount of chemical to which a loss fraction is applied	Value based on Table A-17b	kg/site-day
Freq	The frequency of release of the chemical	Value based on Table A-17c	days/site- year
NS	Number of sites	NS (from Mass Balance Parameters subtab of the Operation Parameters tab)	site(s)
DR	Total daily overspray generation rate to all media	Calculated from model equation	kg/site-day
AR	Total annual overspray generation rate to all media	Calculated from model equation	kg/year (all sites)

You may elect to change any parameter from Table A-17 except the model estimates LF, DR and AR. Clicking the *Type* column for NS contains only two options: the ChemSTEER default from Table A-17 and User-defined. The conditional default and non-default options for TE, Amt and Freq are presented in the tables below. Be sure to read the <u>ChemSTEER Estimation Methods and Models</u> topic for more information about changing model parameters.

## Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled*  Default characterization for Output 1: *Output 1* Default characterization for Output 2: *Output 2* 

You may select an alternative characterization for either of the outputs at any time.

## **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Release Model Information* screen:

"EPA/OPPT Automobile OEM Coating Overspray Loss Model (non-volatiles)"

## Table A-17a. Default and Non-default Values for Coating Transfer Efficiency (TE) for the EPA/OPPT Automobile OEM Coating Overspray Loss Model (non-volatiles)

Spray Gun Type (from the Shared Parameters/Factors subtab of the Operation Parameters tab)	Conditional Default TE (Origin Label)	Non-default Options for TE <sup>1</sup> (Origin Label)
HVLP (High Volume, Low Pressure)	0.65 (HVLP Gun)	0.20 (Conv Gun) User-Defined TE (User Specified)
Conventional <sup>2</sup>	0.20 (Conv Gun)	0.65 (HVLP Gun) User-defined TE (User Specified)

The non-default options for TE may be selected <u>at the model level</u>. If the value for TE is changed in the Releases tab, the new value will only be used in the calculations performed by the model for the selected release source.
 Conventional spray guns are selected as the default for the Automobile OEM Spray Coating operation in the Shared Parameters/ Factors subtab. The conventional spray gun default for the Automobile OEM Spray Coating Operation was adopted as an internal policy decision in July 2003.

Operation Mode/Batch Condition	Operation Type	Mass Balance Basis	Conditional Amt Default (kg/site-day)	Non-default Options for Amt*
Continuous** / Not Applicable	Auto Spray Coating Operations (OEM or Refinish)	Formulated Paint Usage**	DMUchem/DMOchem (kg/site-day) (from Mass Balance Parameters subtab for the Operation Parameters tab)	DMIchem User-defined Amt
		Raw Material (i.e., Purchased Paint Usage	DMIchem (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMUchem User-defined Amt
	Not Auto Spray Coating Operation	Product	DMOchem (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMIchem User-defined Amt
		Raw Material	DMIchem (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMOchem User-defined Amt
Batch / Number of batches per day (Nbd) < 1 (from Mass	Any	Formulated Paint Usage / Product	BMOchem (kg/line-bt) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMIchem x Ls (kg/site-bt) BMOchem x Ls (kg/site-bt) User-defined Amt
Parameters subtab of the Operation Parameters tab)		Purchased Paint Usage / Raw Material	BMIchem (kg/line-bt) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMOchem BMIchem x Ls (kg/site-bt) BMOchem x Ls (kg/site-bt) User-defined Amt
Batch / Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the	Any	Formulated Paint Usage / Product	BMOchem x Nbd (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMOchem BMIchem x Nbd BMIchem x Nbd/Ls (kg/line-day) BMOchem x Nbd/Ls (kg/line-day) User-defined Amt
Operation Parameters tab)		Purchased Paint Usage / Raw Material	BMIchem x Nbd (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMochem BMOchem x Nbd BMIchem x Nbd/Ls (kg/line-day) BMOchem x Nbd/Ls

# Table A-17b. Conditional Default Values for Amt for the EPA/OPPT Automobile OEM Coating Overspray Loss Model (non-volatiles)

					(kg/line-day) User-defined Amt
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\*Non-default options for Amt are available by clicking in the *Type* column in the View/Update Release Model Information screen in the Releases tab.

\*\*Continuous use of formulated paint is the default setting for the Automobile OEM Spray Coating operation on the Mass Balance Parameters subtab.

## Table A-17c. Conditional Default Values for Freq for the EPA/OPPT Automobile OEM Coating Overspray Loss Model (non-volatiles)

Operation Mode	Batch Condition	Conditional Freq Default (days of release/site-yr)	Non-Default Options for Freq*
Continuous**	Not Applicable	OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	User-defined Freq
Batch	Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD User-defined Freq
	Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby User-defined Freq

\*Non-default options for Freq are available by clicking in the *Type* column in the View/Update Release Model Information screen in the Releases tab.

\*\*Continuous is the default setting for the Automobile OEM Spray Coating operation on the Mass Balance Parameters subtab.

## **Key Rationale for Model**

The coating operation generates an overspray release based upon the amount of paint sprayed and the transfer efficiency (TE). This overspray is controlled/contained within a spray booth with a certain control removal efficiency (McE). As defaults, conventional spray guns and booths with waterwash controls are assumed to be used for OEM automobile coating applications. When water type booths are used, the solids removal efficiency (SrE) is not complete. Releases to the various media are estimated based on these three primary parameters.

NOTE: This version of ChemSTEER calculates the daily overspray generation amounts only and assumes that releases occur when the generation occurs. Future ChemSTEER versions will allow the calculation of water purges and solids releases to other media at different release frequencies.

## Reference

SAIC for US EPA/OPPT. Generic Scenario for Automobile Spray Coating Draft Report. August 1996.

Organization for Economic Co-operation and Development. Emission Scenario Document on Coating Application via Spray Painting in the Automotive Refinishing Industry. June 2010.

#### EPA/OPPT Automobile Refinish Coating Overspray Loss Model

#### **Model Description**

This model estimates releases of overspray of non-volatile chemical in coatings during their application to refinished automobiles using spray guns within a spray booth with controls to capture overspray from the exhaust.

#### Sources/Activities That Use This Model as a Default

The EPA/OPPT Automobile Refinish Coating Overspray Loss Model is the default for calculating multi-media releases of a chemical to air, as well as water, incineration, or landfill for the <u>Automobile</u> <u>Refinish Spray Coating Application</u> source/activity.

#### EPA/OPPT Automobile Refinish Coating Overspray Loss Model – Other Sources/Activities

The EPA/OPPT Automobile Refinish Coating Overspray Loss Model may be an appropriate alternative to the default release model for the following sources/activities:

- <u>Coating Using Hand Held Spray Gun</u>
- <u>Coating Using Hand Held Spray Can</u>

#### **Potential Media of Release**

Air, Incineration, Landfill and/or Water (see Default Media of Release section below)

#### **Default Media of Release**

% to Air = (1-McE) × 100 % to Water = McE × (1- SrE) × 100 % to Landfill or Incineration = McE × SrE × 100

NOTE: If you change the value(s) of McE and/or SrE and click *OK* in the *View / Update Release Model Information* screen, the values of the percent to each medium of release will be automatically updated according to the above equations. If you had previously changed the media of release designations to non-default percentages, the changes will be overwritten, and you will need to return to the Modify Media of Release window to re-enter your changes.

#### Equations

For daily releases:

DR (kg/site-day) = LF × Amt DR occurs over [Freq] days/year For annual releases:

AR (kg/year) = DR × Freq × NS, AR is for all sites combined

## Model Input Parameters and Default Values

The EPA/OPPT Automobile Refinish Coating Overspray Loss Model (non-volatiles) default values for each of the input parameters are summarized in Table A-18.

Parameter	Description	Default Value(s)	Units
LF	Loss fraction; fraction of an amount of the chemical that is estimated to be released	1-TE	dimensionless
TE	Spray gun transfer efficiency	<i>Output 1:</i> <u>Default:</u> 0.2 (conventional gun default) <u>Non-default option:</u> User-defined TE (see Table A-18a)	dimensionless
		<i>Output 2:</i> <u>Default:</u> 0.2 (conventional gun default) <u>Non-default option:</u> User-defined TE (see Table A-18a)	
McE	Spray mist capture efficiency	Output 1: <u>Default:</u> 0.96 (dry filter/waterwash default) <u>Non-default options:</u> User-defined McE	dimensionless
		Output 2: <u>Default:</u> 0.96 (dry filter/waterwash default) <u>Non-default option:</u> User-defined McE	
SrE	Solid removal efficiency from captured mist	Output 1: <u>Default:</u> 1 (dry filter default) <u>Non-default option:</u> 0.90 (waterwash); and User-defined SrE	dimensionless
		Output 2: <u>Default:</u> 1 (dry filter default) <u>Non-default option:</u> 0.90 (waterwash); and User-defined SrE	
Amt	The amount of chemical to which a loss fraction is applied	Value based on Table A-18b	kg/site-day
Freq	The frequency of release of the chemical	Value based on Table A-18c	days/site- year
NS	Number of sites	NS (from Mass Balance Parameters subtab of the Operation Parameters tab)	site(s)
DR	Total daily overspray generation rate to all media	Calculated from model equation	kg/site-day
AR	Total annual overspray generation rate to all media	Calculated from model equation	kg/year (all sites)

# Table A-18. Input Parameters and Default Values for the EPA/OPPT Automobile Refinish Coating Overspray Loss Model (non-volatiles)

You may elect to change any parameter from Table A-18 except the model estimates LF, DR and AR. Clicking the *Type* column for NS contains only two options: the ChemSTEER default from Table A-18 and User-defined. The conditional default and non-default options for TE, Amt and Freq are presented in the tables below. Be sure to read the <u>ChemSTEER Estimation Methods and Models</u> topic for more information about changing model parameters.

## Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Enabled* Enable Model Parameters for Output 2: *Enabled* 

Default characterization for Output 1: *Typical* Default characterization for Output 2: *Worst-Case* 

You may select an alternative characterization for either of the outputs at any time.

## **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Release Model Information* screen:

"EPA/OPPT Automobile Refinish Coating Overspray Loss Model (non-volatiles)"

## Table A-18a. Default and Non-default Values for Coating Transfer Efficiency (TE) for the EPA/OPPT Automobile Refinish Coating Overspray Loss Model (non-volatiles)

Spray Gun Type (from the Shared Parameters/Factors subtab of the Operation Parameters tab)	Conditional Default TE (Origin Label)	Non-default Options for TE <sup>1</sup> (Origin Label)
HVLP (High Volume, Low Pressure)	0.65 (HVLP Gun)	0.20 (Conv Gun) User-Defined TE (User Specified)
Conventional <sup>2</sup>	0.20 (Conv Gun)	0.65 (HVLP Gun) User-defined TE (User Specified)

The non-default options for TE may be selected <u>at the model level</u>. If the value for TE is changed in the Releases tab, the new value will only be used in the calculations performed by the model for the selected release source.
 Conventional spray guns are selected as the default for the Automobile Refinish Spray Coating operation in the Shared Parameters/ Factors subtab.

Operation Mode/Batch Condition	Operation Type	Mass Balance Basis	Conditional Amt Default (kg/site-day)	Non-default Options for Amt*
Continuous** / Not Applicable	Auto Spray Coating Operations (OEM or Refinish)	Formulated Paint Usage**	DMUchem/DMOchem (kg/site-day) (from Mass Balance Parameters subtab for the Operation Parameters tab)	DMIchem User-defined Amt
		Purchased Paint Usage** (i.e., Raw Material)	DMIchem (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMUchem User-defined Amt
	Not Auto Spray Coating Operation	Product	DMOchem (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMIchem User-defined Amt
		Raw Material	DMIchem (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMOchem User-defined Amt
Batch / Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Any	Formulated Paint Usage / Product	BMOchem (kg/line-bt) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMIchem x Ls (kg/site-bt) BMOchem x Ls (kg/site-bt) User-defined Amt
		Purchased Paint Usage / Raw Material	BMIchem (kg/line-bt) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMOchem BMIchem x Ls (kg/site-bt) BMOchem x Ls (kg/site-bt) User-defined Amt
Batch / Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the	Any	Formulated Paint Usage / Product	BMOchem x Nbd (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMOchem BMIchem x Nbd BMIchem x Nbd/Ls (kg/line-day) BMOchem x Nbd/Ls (kg/line-day) User-defined Amt
Operation Parameters tab)		Purchased Paint Usage / Raw Material	BMIchem x Nbd (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIchem BMochem BMOchem x Nbd BMIchem x Nbd/Ls (kg/line-day) BMOchem x Nbd/Ls

# Table A-18b. Conditional Default Values for Amt for the EPA/OPPT Automobile Refinish Coating Overspray Loss Model (non-volatiles)

|--|

\*Non-default options for Amt are available by clicking in the *Type* column in the View/Update Release Model Information screen in the Releases tab.

\*\*Continuous use of purchased paint is the default setting for the Automobile Refinish Spray Coating operation on the Mass Balance Parameters subtab.

## Table A-18c. Conditional Default Values for Freq for the EPA/OPPT Automobile Refinish Coating Overspray Loss Model (non-volatiles)

Operation Mode	Batch Condition	Conditional Freq Default (days of release/site-yr)	Non-Default Options for Freq*
Continuous**	Not Applicable	OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	User-defined Freq
Batch	Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD User-defined Freq
	Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby User-defined Freq

\*Non-default options for Freq are available by clicking in the Type column in the View/Update Release Model Information screen in the Releases tab.

\*\*Continuous is the default setting for the Automobile Refinish Spray Coating operation on the Mass Balance Parameters subtab.

## Key Rationale for Model

The coating operation generates an overspray release based upon the amount of paint sprayed and a transfer efficiency (TE). This overspray is controlled/contained within a spray booth with a certain control removal efficiency (MCE). As defaults, conventional spray guns and booths with dry filters are assumed to be used for automobile refinish coating applications. When water type booths are used, the solids removal efficiency (SrE) is not complete. Releases to the various media are estimated based on these three primary parameters.

NOTE: This version of ChemSTEER calculates the daily overspray generation amounts only and assumes that releases occur when the generation occurs. Future ChemSTEER versions will allow the calculation of water purges and solids releases to other media at different release frequencies.

## Reference

Organization for Economic Co-operation and Development. Emission Scenario Document on Coating Application via Spray Painting in the Automotive Refinishing Industry. June 2010.

## EPA/OPPT Electroplating Rinse Water Loss Model

## **Model Description**

This model estimates the releases of additives due to rinses of parts removed from the electroplating baths. The rinse water is treated to recover usable additives that are returned to the baths. The additives that are not recovered are expected to be discharged to on-site treatment, where additives are expected to partition to wastewater and sludge, which is assumed to be sent to land or incineration disposal.

**NOTE**: This model is the default model for estimating releases to water and land/incineration from the <u>Rinsing Electroplated Parts</u> source/ activity. This model may not be used for any other source/activity in ChemSTEER.

## **Potential Media of Release**

Air, Incineration, Land and/or Water (see Default Media of Release section below)

## **Default Media of Release**

% to Water = (1- WWTE) x 100

% to Land or Incineration = WWTE x 100

**NOTE:** If you change the value of WWTE and click *OK* in the *View / Update Release Model Information* screen, the values of the percent to each medium of release will be automatically updated according to the above equations. If you had previously changed the media of release designations to non-default percentages, the changes will be overwritten, and you will need to return to the Modify Media of Release window to re-enter your changes.

## Equations

For daily releases:

DR (kg/site-day) = DVrinse x 3.78 L/gal x Yrinse x Drinse x (1 - RinseE)

DR occurs over [Freq] days/year

For annual releases:

AR (kg/year) = DR x Freq x NS, AR is for all sites combined

## **Model Input Parameters and Default Values**

The EPA/OPPT Electroplating Rinse Water Loss Model default values for each of the input parameters are summarized in Table A-19.

Parameter	Description	Default Value(s)	Units
DVrinse	Daily volume of rinsewater generated per site	DVrinse (from Mass Balance Parameters subtab of Operation Parameters tab) (default: 4,932)	gal/site-day
Drinse	Density of the rinse water	Drinse (from Mass Balance Parameters subtab of Operation Parameters tab) (default: 1)	kg/L
Yrinse	Concentration of PMN in rinse water	Yrinse (from Mass Balance Parameters subtab of Operation Parameters tab) (default: 0.0235)	dimensionless
RinseE	Rinse water recovery efficiency	RinseE (from Mass Balance Parameters subtab of Operation Parameters tab) (default: 0.9)	dimensionless
WWTE	Wastewater treatment efficiency	Value based on Table A-19a	dimensionless
Freq	The frequency of release of the chemical	OD (from Mass Balance Parameters subtab of Operation Parameters tab)	day/site-year
NS	Number of sites	NS (from Mass Balance Parameters subtab of Operation Parameters tab)	site(s)
DR	Total daily release	Calculated from model equation	kg/site-day
AR	Total annual release	Calculated from model equation	kg/year (all sites)

## Table A-19. Input Parameters and Default Values for the EPA/OPPT Electroplating Rinse Water Loss Model

You may not change the value of the any parameter from Table A-19 except WWTE. Clicking the *Type* column for WWTE launches a window that displays the conditional default and non-default options, which are shown in Table A-19a. Be sure to read the <u>ChemSTEER Estimation Methods and</u> <u>Models</u> topic for more information about changing model parameters.

## Default Parameter Value Switch Settings and Results Characterization:

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default characterization for Output 1: *Output 1* Default characterization for Output 2: *Output 2* 

You may select an alternative characterization for either of the outputs at any time.

## Default Model Basis:
The following default text is displayed in the *Basis* box on the *View/Update Release Model Information* screen:

"EPA/OPPT Electroplating Rinse Water Loss Model"

# Table A-19a. Default and Non-default Values for Wastewater Treatment Efficiency (WWTE) for the EPA/OPPT Electroplating Rinse Water Loss Model

Electroplating Additive Type (from the Shared Parameters/Factors subtab of the Operation Parameters tab)	Conditional Default WWTE (Origin Label)	Non-Default Options for WWTE <sup>1</sup> (Origin Label)
Suspended Solids	0.97 (Suspended Solids)	0.5 (Organic Compounds) User-defined TE (User Specified)
Organic Compounds <sup>2</sup>	0.5 (Organic Compounds)	0.97 (Suspended Solids) User-Defined TE (User-Specified)

1. The non-default options for WWTE may be selected <u>at the model level</u>. If the value for WWTE is changed in the *Releases* tab, the new value will only be used in the calculations performed by the model for the selected release source. To maintain consistency for all models, you should only change WWTE in the *Shared Parameters/ Factors* subtab.

2. Organic compounds are selected as a worst case default in the Shared Parameters/Factors subtab.

#### **Key Rationale for Model**

Rinse water is treated and 90% of the additives are recovered and returned to the electroplating baths. The additives that are not recovered are assumed to be discharged to on-site treatment, where additives are expected to partition to wastewater and sludge, which is assumed to be sent to land or incineration disposal.

#### Reference

SAIC for US EPA/OPPT. Generic Scenario: Electroplating. August 1996.

### EPA/OPPT Electroplating Spent Bath Disposal Model

#### **Model Description**

This model estimates the releases of additives due to periodic disposal of spent electroplating baths. The baths are discharged to on-site treatment, where additives in the baths are expected to partition to wastewater and sludge, which is assumed to be sent to land or incineration disposal.

NOTE: This model is the default model for estimating releases to water and land/incineration from the <u>Changing Electroplating Bath</u> source/ activity. This model may not be used for any other source/activity in ChemSTEER.

#### **Potential Media of Release**

Air, Incineration, Land and/or Water (see Default Media of Release section below)

#### **Default Media of Release**

% to Water = (1- WWTE) x 100 % to Land or Incineration = WWTE x 100

NOTE: If you change the value of WWTE and click *OK* in the *View / Update Release Model Information* screen, the values of the percent to each medium of release will be automatically updated according to the above equations. If you had previously changed the media of release designations to non-default percentages, the changes will be overwritten, and you will need to return to the Modify Media of Release window to re-enter your changes.

#### Equations

For daily releases: DR (kg/site-day) = (DVbath x 3.78L/gal x Ybath x Dbath) DR occurs over [Freq] days/year

For annual releases: AR (kg/year) = DR x Freq x NS, AR is for all sites combined

#### **Model Input Parameters and Default Values**

The EPA/OPPT Electroplating Spent Bath Disposal Model default values for each of the input parameters are summarized in Table A-20.

Parameter	Description	Default Value(s)	Units
DVbath	Daily volume of bath change	Vbath x Nbath (from Mass Balance Parameters subtab of Operation Parameters tab) (default: 2,500 x 3 = 7,500) Non-default option*: Vbath	gallons
Dbath	Density of the bath	Dbath (from Mass Balance Parameters subtab of Operation Parameters tab) (default: 1)	kg/L
Ybath	Concentration of chemical in bath	Ybath (from Mass Balance Parameters subtab of Operation Parameters tab) (default: 0.0434)	dimensionless
WWTE	Wastewater treatment efficiency	Value based on Table A-20a	dimensionless
Freq	The frequency of release of the chemical	Freqbath (from Mass Balance Parameters subtab of Operation Parameters tab) (default: 2) Non-default option*: Freqbath x Nbath	day/site-year
NS	Number of sites	NS (from Mass Balance Parameters subtab of Operation Parameters tab)	site(s)
DR	Total daily release	Calculated from model equation	kg/site-day
AR	Total annual release	Calculated from model equation	kg/year (all sites)

## Table A-20. Input Parameters and Default Values for the EPA/OPPT Electroplating Spent Bath Disposal Model

\* ChemSTEER automatically "pairs" the default and non-default options for DVbath and Freq. If you select the default for one parameter, the default of the other parameter is used. If you select the non-default of one parameter, the non-default of the other parameter is used.

You may change the values of the following parameters from Table A-20: DVbath and Freq ("paired" default and non-default options only as specified in Table A-20) and WWTE. Clicking the *Type* column for any of these changeable parameters launches a window that displays the options. The conditional default and non-default options for WWTE are presented in Table A-20a. Be sure to read the <u>ChemSTEER Estimation Methods and Models</u> topic for more information about changing model parameters.

#### Default Parameter Value Switch Settings and Results Characterization:

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default characterization for Output 1: *Output 1* Default characterization for Output 2: *Output 2* 

You may select an alternative characterization for either of the outputs at any time.

#### Default Model Basis:

The following default text is displayed in the *Basis* box on the *View/Update Release Model Information* screen:

"EPA/OPPT Electroplating Spent Bath Disposal Model"

# Table A-20a. Default and Non-default Values for Wastewater Treatment Efficiency (WWTE) for the EPA/OPPT Electroplating Spent Bath Disposal Model

Electroplating Additive Type (from the Shared Parameters/Factors subtab of the Operation Parameters tab)	Conditional Default WWTE (Origin Label)	Non-Default Options for WWTE <sup>1</sup> (Origin Label)
Suspended Solids	0.97 (Suspended Solids)	0.5 (Organic Compounds) User-defined TE (User Specified)
Organic Compounds <sup>2</sup>	0.5 (Organic Compounds)	0.97 (Suspended Solids) User-Defined TE (User-Specified)

1. The non-default options for WWTE may be selected <u>at the model level</u>. If the value for WWTE is changed in the *Releases* tab, the new value will only be used in the calculations performed by the model for the selected release source. To maintain consistency for all models, you should only change WWTE in the *Shared Parameters/ Factors* subtab.

2. Organic compounds are selected as a worst case default in the Shared Parameters/ Factors subtab.

#### Key Rationale for Model

This model assumes that releases of additives occur due to semi-annual, simultaneous (as default) disposal of spent electroplating baths. The model assumes that the entire volume of each bath tank is disposed. The spent baths are assumed to be discharged to on-site treatment, where additives in the baths are expected to partition to wastewater and sludge, which is assumed to be sent to land or incineration disposal.

#### Reference

SAIC for US EPA/OPPT. Generic Scenario: Electroplating. August 1996.

#### Models for Calculating Releases of Liquids

#### Releases Due to Evaporation

The following models may be selected for sources/activities that result in releases due to evaporation:

- <u>EPA/OPPT Mass Transfer Coefficient Model</u>
- <u>EPA/OPPT Penetration Model</u>
- EPA/OPPT Cooling Tower Evaporative Loss Model (volatiles)
- <u>User-Defined Vapor Generation Rate Model</u>
- User-Defined Loss Rate Model

## Releases During Container Filling (Vapor Displacement)

The following models may be selected for sources/activities that result in releases during container filling:

- EPA/OAQPS AP-42 Loading Model
- <u>User-Defined Vapor Generation Rate Model</u>
- User-Defined Loss Rate Model

### Releases of Residual and Waste Liquids

The following models may be selected for sources/activities that result in releases of residual and waste liquids:

- <u>EPA/OPPT Bulk Transport Residual Model</u>
- EPA/OPPT Drum Residual Model
- EPA/OPPT Multiple Process Vessel Residual Model
- EPA/OPPT Single Vessel Residual Model
- EPA/OPPT Small Container Residual Model
- EPA/OPPT Water Saturation Loss Model
- EPA/OPPT Automobile OEM Coating Overspray Loss Model
- <u>EPA/OPPT Automobile Refinish Coating Overspray Loss Model</u>
- <u>EPA/OPPT Cooling Tower Blowdown Loss Model</u>
- EPA/OPPT Cooling Tower Windage Loss Model
- EPA/OPPT Electroplating Rinse Water Loss Model
- EPA/OPPT Electroplating Spent Bath Disposal Model
- User-Defined Loss Rate Model

#### Models for Calculating Releases of Solids

#### Releases of Residual Solids

The following models may be selected for sources/activities that result in releases of residual solids:

- <u>EPA/OPPT Solid Residuals in Transport Containers Model</u>
- EPA/OPPT Solids Transfer Dust Loss Model
- User-Defined Loss Rate Model

## **WORKER EXPOSURES**

#### General Guidelines for Exposure Assessment

Detailed descriptions of the worker exposure models are contained in several User Guide topics, organized according to the type of exposure (e.g., inhalation or dermal), the form of the substance (e.g., liquid or solid material), and models that utilize exposure limits as the basis for the calculation. Simply click on the desired grouping of models in the User Guide Table of Contents to access these detailed descriptions.

Each manufacturing, processing, and use operation to be assessed are analyzed to determine the sources/ activities that can result in worker exposures that are to be estimated. Once these sources/ activities are identified, a general hierarchy of preference may be used to determine how to quantify each exposure from each source/ activity. The following list shows the potential methods for quantifying exposures in order (generally) from the most preferred to the least preferred.

- 1. Measured personal exposure monitoring data for the chemical.
- 2. "Indirectly" measured area exposure concentration monitoring data.
- 3. Measured data for a "surrogate" chemical with similar "exposure-affecting" properties and used in the same (or very similar) process.
- 4. Modeled exposure estimates:
  - Simulated exposure estimates (e.g., mass balance model) for the chemical.
  - Regulated limits as an estimated "upper bound" of exposure.
  - "Rule-of-thumb" exposure estimates, or those developed using analogous points of reference and engineering judgment.

This order of preference is expected to apply generally to most cases of worker exposure assessment. However, judgment may dictate that, in some cases, the order within the hierarchy should be changed. Examples of such a change of hierarchy order may include when data are judged to be unreliable or unrepresentative for a particular reason. Also, some estimates may be a combination of two or more of these methods.

Estimation methods in ChemSTEER are based on a combination of factors:

- research and knowledge of and data from unit operations and industrial processes,
- some basic chemical engineering principles,
- professional experience and judgment.

Standard methods and models in ChemSTEER have been developed to estimate worker exposures for a variety of industrial and commercial operations.

#### Quick Summary of ChemSTEER Inhalation Exposure Models

All of the ChemSTEER inhalation exposure models are summarized in the table below. For each model, a brief description of the primary calculation(s), as well as a list of the ChemSTEER worker

activities (or activity categories) that use the model as the default for calculating exposures, are provided.

**NOTE**: This table is intended to provide you a "snapshot" of the various ChemSTEER models to help you become more familiar with them. You are highly encouraged to review the full description of the models (provided in this section of the User Guide), as well as the source/activity topics (provided in the <u>Release Sources and Exposure Activities</u> section of the User Guide), for a more complete description of the calculations and logic used.

Quick Summary of ChemSTEER Inhalation Exposure Models		
Inhalation Exposure Model	Brief Description of Calculation or Basis of the Inhalation Potential Dose Rate (mg/day) [I=Cm x b x h]	Activities That Use the Model as a Default for Calculating Exposures
<i>Models for Calculating Worker Inhalatio</i> NOTE: These models only appear as defai handled is within the specified AVP range	n Exposure to a Chemical Vapor ults for calculating exposures to a volatile chemical (i. .).	e., the adjusted vapor pressure (AVP) of the material being
EPA/OPPT Mass Balance Inhalation Model	Cm = mass concentration of the chemical in air (mg/m <sup>3</sup> ) = Cv x MW/Vm Where: Cv = volumetric concentration of the chemical in air (ppm) (uses model equation that utilizes G* (vaporization rate (g/s)) and other shared parameters) MW = molecular weight of the chemical (g/mol) Vm = molar volume (L/mol) (default: 24.45 @ 25 °C and 1 atm) b = volumetric inhalation rate (m <sup>3</sup> /hr) (default: 1.25) h* = exposure duration (hrs/day) *You must select and run a corresponding vapor generation <u>release</u> model for the activity in order to obtain appropriate default values for the G and h parameters. Be sure to read this model's User Guide topic for more information.	Loading Liquids into Transport Containers/Vessels (all activity types) Unloading Liquids from Transport Containers/Vessels (all activity types) Cleaning Liquid Residuals from Transport Containers/Vessels (all activity types) Sampling Liquids (all activity types) Vapor Release from Open Liquid Surfaces
OSH PEL-Limiting Model for Substance Specific Vapors	Cm = mass concentration of the chemical in air (mg/m <sup>3</sup> ) =Cv x MW/Vm	There are no activities that use this model as a default for calculating worker inhalation of the chemical vapor.

	Where: Cv* = volumetric concentration in air (ppm) (uses model equation that utilizes user-input values for several parameters, including a concentration limit (e.g., PEL)) MW = molecular weight of the chemical (g/mol) Vm = molar volume (L/mol) (default: 24.45 @ 25 °C and 1 atm) b = volumetric inhalation rate (m <sup>3</sup> /hr) (default: 1.25) h = exposure duration (hrs/day) (default: 8) *Be sure to read this model's User Guide topic for more information	NOTE: You may choose this model for any <u>volatile liquid-handling</u> activity for which you wish to base the exposure estimates on a known permissible limit.
Models for Calculating Worker Inhalatio	n Exposures to a Chemical Mist	
OSHA Total PNOR PEL-Limiting Model	Cm = mass concentration of the chemical in air (mg/m <sup>3</sup> ) = KCk x Ys Where: KCk = mass concentration limit of total particulate in air (mg/m <sup>3</sup> ) (default: 15) Ys = weight fraction of the chemical in the airborne particulate b = volumetric inhalation rate (m <sup>3</sup> /hr) (default: 1.25) h = exposure duration (hrs/day) (default: 8)	Coating Using Hand-Held Spray Gun NOTE: This model is also the default model for several solids processing activities. Please refer to the <i>Chemical Dust</i> <i>Exposure</i> section of this table for a list of those activities.
OSHA Respirable PNOR PEL-Limiting	Cm = mass concentration of the chemical in air	There are no activities that use this model as a default for

Model	(mg/m³)	calculating worker inhalation of the chemical mist.
	= KCk x Ys	
		NOTE: You may choose this model for any fine mist-generating
	Where:	activity for which you wish to base the exposure estimates on
	KCk = mass concentration limit of total	the generic permissible limit for <u>respirable</u> particles.
	particulate in air (mg/m <sup>3</sup> ) (default: 5)	
	, , , , ,	
	Ys = weight fraction of the chemical in the	
	airborne particulate	
	h = volumetric inhalation rate (m3/hr) (default:	
	1 25)	
	1.25)	
	h = exposure duration (hrs/day) (default: 8)	
	Concernence and the state of the share in the state of th	On anothing the Electronylating Dath User OCUA DEL for sharesing
OSHA PEL-LIMITING Model for	Cm = mass concentration of the chemical in air	Operating the Electroplating Bath Uses OSHA PEL for chromium
Substance-Specific Particulates	(mg/m <sup>*</sup> )	(KCk=0.5 mg/m <sup>-</sup> ) and est. chromium batch concentration
	= KCk x Ys/Ypel	(Ypel=0.25) as overriding defaults.
	Where:	NOTE: You may choose this model for any <u>mist-generating</u>
	KCk = mass concentration limit of total	activity for which you wish to base the exposure estimates on a
	particulate in air (mg/m <sup>2</sup> ) (default: 15, but you	known permissible limit.
	may enter a PEL for a known chemical	
	substance in the mist)	
	Ys = weight fraction of the chemical in the	
	airborne particulate	
	Ypel = weight fraction of the substance in the	
	mist for which the PEL is known	
	b = volumetric inhalation rate (m <sup>3</sup> /hr) (default:	
	1.25)	
	h = exposure duration (hrs/day) (default: 8)	
EPA/OPPT UV Roll-Coating Inhalation	Cm = mass concentration of the chemical in air	Roll Coating
Model	$(mg/m^3)$	Ŭ
	= KCk x Ys	

	<ul> <li>Where: KCk = mass concentration of total particulate in air (mg/m<sup>3</sup>) (default: between 0.04 and 0.26)</li> <li>Ys = Lesser of Ymist/Ysf or 1; Ymist = weight fraction of the chemical in the mist; Ysf = weight fraction of solids/non-volatile components in the mist</li> <li>b = volumetric inhalation rate (m<sup>3</sup>/hr) (default: 1.25)</li> <li>h = exposure duration (hrs/day) (default: 8)</li> </ul>	
Models for Calculating Worker Inhalatio	n Exposures to a Chemical Dust	
EPA/OPPT Small Volume Handling Model	Inhalation Dose Rate (I) = EF x AH x Ys x Sd Where: EF = exposure factor (mg/kg) (default: between 0.0477 and 0.161) AH = amount of solids containing the chemical being handled in the activity (kg/worker-shift)	Sampling Solids (all activity types) This model also may be the default for the following activities, <u>if the amount of solids being handled is &lt; 54 kg/worker-day:</u> <u>Loading Solids</u> into Transport Containers/Vessels (all activity types) <u>Unloading Solids</u> from Transport Containers/Vessels (all activity
	Ys = weight fraction of the chemical in the dust Sd = number of shifts per worker, per day	types) Cleaning <u>Solid Residuals</u> from Transport Containers/Vessels (all activity types) Equipment Cleaning Losses of <u>Solids</u> Miscellaneous Activities Related to <u>Solid Processing</u>
OSHA Total PNOR PEL-Limiting Model	Cm = mass concentration of the chemical in air (mg/m <sup>3</sup> ) = KCk x Ys	Grinding and Sanding This model may also be the default for the following activities, <u>if the amount of solids being handled is &gt; 54 kg/worker-day.</u>

	Where: KCk = mass concentration limit of total particulate in air (mg/m <sup>3</sup> ) (default: 15)	<u>Loading Solids</u> into Transport Containers/vessels (all activity types)
	Ys = weight fraction of the chemical in the airborne particulate	<u>Unloading Solids</u> from Transport Containers/Vessels (all activity types)
	b = volumetric inhalation rate (m <sup>3</sup> /hr) (default: 1.25)	Equipment Cleaning Losses of <u>Solids</u>
	h = exposure duration (hrs/day) (default: 8)	Miscellaneous Activities Related to Solid Processing
		NOTE: This model is also the default model for mist-producing activities. Please refer to the <i>Chemical Mist Exposure</i> section of this table for a list of those activities.
OSHA Respirable PNOR PEL-Limiting Model	Cm = mass concentration of the chemical in air (mg/m <sup>3</sup> ) = KCk x Ys	There are no activities that use this model as a default for calculating worker inhalation of the chemical dust.
		NOTE: You may choose this model for any fine dust-generating
	Where:	activity for which you wish to base the exposure estimates on
	particulate in air $(mg/m^3)$ (default: 5)	the generic permissible limit for <u>respirable</u> particles.
	Ys = weight fraction of the chemical in the airborne particulate	
	b = volumetric inhalation rate (m <sup>3</sup> /hr) (default: 1.25)	
	h = exposure duration (hrs/day) (default: 8)	
OSHA PEL-Limiting Model for Substance-Specific Particulates	Cm = mass concentration of the chemical in air (mg/m <sup>3</sup> ) = KCk x Ys/Ypel	There are no activities that use this model as a default for calculating worker inhalation of the chemical dust.
		NOTE: You may choose this model for any <u>dust-generating</u>
	Where: KCk = mass concentration limit of total	activity for which you wish to base the exposure estimates on a known permissible limit.
	particulate in air (mg/m <sup>3</sup> ) (default: 15, but you may enter a PEL for a known chemical	

	substance in the dust)	
	Ys = weight fraction of the chemical in the airborne particulate	
	Ypel = weight fraction of the substance in the mist for which the PEL is known	
	b = volumetric inhalation rate (m <sup>3</sup> /hr) (default: 1.25)	
	h = exposure duration (hrs/day) (default: 8)	
EPA/OPPT UV Roll-Coating Inhalation Model	Cm = mass concentration of the chemical in air (mg/m <sup>3</sup> ) = KCk x Ys	Roll Coating
	Where: KCk = mass concentration of total particulate in air (mg/m <sup>3</sup> ) (default: between 0.04 and 0.26)	
	Ys = lesser of Ymist/Ysf or 1; Ymist = weight fraction of the chemical in the mist; Ysf = weight fraction of solids/non-volatile components in the mist	
	b = volumetric inhalation rate (m <sup>3</sup> /hr) (default: 1.25)	
	h = exposure duration (hrs/day) (default: 8)	
Models for Calculating Exposures During	Industry-Specific Activities	
EPA/OPPT Automobile OEM Spray Coating Inhalation Exposure Model (non-volatile non-polyisocyanates)	Cm = mass concentration of the chemical in air (mg/m <sup>3</sup> ) = KCk x Ys	Automobile <u>OEM</u> Spray Coating Application
(used in the Automobile OEM Spray Coating operation)	Where: KCk = mass concentration of total particulate	

	in air (mg/m <sup>3</sup> ) (default: 2.3, based on spray gun type and spray booth ventilation type)	
	Ys = lesser of Ymist/Ysf or 1; Ymist = weight fraction of the chemical in the mist; Ysf = weight fraction of solids/non-volatile components in the mist	
	b = volumetric inhalation rate (m <sup>3</sup> /hr) (default: 1.25)	
	h = exposure duration (hrs/day) (default: 8)	
EPA/OPPT Automobile Refinish Spray Coating Inhalation Exposure Model (non-volatile non-polyisocyanates)	Cm = mass concentration of the chemical in air (mg/m <sup>3</sup> ) = KCk x Ys	Automobile <u>Refinish</u> Spray Coating Application
(used in the Automobile Refinish Spray Coating operation)	Where: KCk = mass concentration of total particulate in air (mg/m <sup>3</sup> ) (default: 15, based on spray gun type and spray booth ventilation type)	
	Ys = lesser of Ymist/Ysf or 1; Ymist = weight fraction of the chemical in the mist; Ysf = weight fraction of solids/non-volatile components in the mist	
	b = volumetric inhalation rate (m <sup>3</sup> /hr) (default: 1.25)	
	h = exposure duration (hrs/day) (default: 8)	
EPA/OPPT Automobile Spray Coating Inhalation Exposure Model (non- volatile polyisocyanates)	Cm = mass concentration of the chemical in air (mg/m <sup>3</sup> ) = KCk	There are no activities that use this model as a default for calculating worker inhalation of the chemical overspray mists/dusts.
(can be used in either of the Automobile Spray Coating operations)	Where: KCk = mass concentration of polyisocyanate mists/dusts in air (mg/m³) (default is based on	NOTE: It is recommended that you substitute this model for the default inhalation model in either of the Automobile Spray Coating operations if the chemical being assessed is a

	spray gun type and spray booth ventilation type; ranges between 0.01 and 18.4)	polyisocyanate compound.
	b = volumetric inhalation rate (m <sup>3</sup> /hr) (default: 1.25)	
	h = exposure duration (hrs/day) (default: 8)	
Models for Calculating During Other Gen	neric Unit Operations	
User-Defined Inhalation Model	Cm = mass concentration of the chemical in air $(mg/m^3)$	Aqueous Wash of Organic Mass
(can be used to estimate exposures to a chemical vapor or particulate/mist)	=Cv x MW/Vm x Ys	Scrubber Releases
	Where: Cv* = volumetric concentration in air (ppm)	Coating Using Hand-Held Spray Can
	(uses model equation that utilizes user-input values for several parameters, including a	Miscellaneous Activities Related to Liquid Processing
	volumetric concentration)	NOTE: You may choose this model for any activity for which you wish to base the exposure estimates on a known
	MW = molecular weight of the chemical (g/mol)	volumetric airborne concentration of the chemical.
	Vm = molar volume (L/mol) (default: 24.45 @ 25 °C and 1 atm)	
	Ys = weight fraction of the chemical in the mixture (default: 1)	
	b = volumetric inhalation rate (m <sup>3</sup> /hr) (default: 1.25)	
	h* = exposure duration (hrs/day)	
	*If assessing an exposure to a chemical <u>vapor</u> , it is recommended that you select and run a corresponding vapor generation <u>release</u> model for the activity in order to obtain appropriate default values for several of the parameters. Be	

sure to read this model's User Guide topic for	
more information.	

### Quick Summary of ChemSTEER Dermal Exposure Models

All of the ChemSTEER dermal exposure models are summarized in the table below. For each model, a brief description of the primary calculation(s), as well as a list of the ChemSTEER worker activities (or activity categories) that use the model as the default for calculating exposures, is provided.

**NOTE**: This table is intended to provide you a "snapshot" of the various ChemSTEER models to help you become more familiar with them. You are highly encouraged to review the full description of the models (provided in this section of the User Guide), as well as the source/activity topics (provided in the <u>Release Sources and Exposure Activities</u> section of the User Guide), for a more complete description of the calculations and logic used.

	Quick Summary of ChemSTEER Dermal Exposure Models			
Dermal Exposure Model	Brief Description of Calculation or Basis of Dermal Potential Dose Rate (mg/day) [Dexp = S x Qu x Yderm x FT]	Activities That Use the Model as a Default for Calculating Exposures		
Models for Calculating Worker De	rmal Exposures to a Liquid Chemical			
EPA/OPPT 1-Hand Dermal Contact with Liquid Model	S = surface area of contact (cm <sup>2</sup> ) (default: 535 for one hand)	Sampling Liquids (all activity types)		
	Qu = quantity remaining on skin (mg/cm <sup>2</sup> -event) (default: ranges between 0.7 and 2.1)			
	Yderm = weight fraction of chemical in the liquid			
	FT = frequency of events (events/worker-day) (default: 1)			
EPA/OPPT 2-Hand Dermal Contact with Liquid Model	S = surface area of contact (cm <sup>2</sup> ) (default: 1,070 for two hands)	Loading Liquids into Transport Containers/Vessels (all activity types)		
	Qu = quantity remaining on skin	<u>Unloading</u> Liquids from Transport Containers/Vessels (all activity types)		
	(mg/cm <sup>2</sup> -event) (default: ranges between 0.7 and 2.1)	<u>Cleaning</u> Liquid Residuals from Transport Containers/Vessels (all activity types)		
		Aqueous Wash of Organic Mass		
	Yderm = weight fraction of chemical in the liquid	Liquid/Liquid Extraction Solvent Disposal		
	FT = frequency of events (events/worker-day) (default: 1)			
EPA/OPPT 2-Hand Dermal Immersion in Liquids Model	S = surface area of contact (cm <sup>2</sup> ) (default: 1,070 for two hands)	Miscellaneous Activities Related to Liquid Processing		
	Qu = quantity remaining on skin (mg/cm <sup>2</sup> -event) (default: ranges between 1.3 and 10.3)	Automobile OEM Spray Coating Application (used in the Automobile OEM Spray Coating Operation) Automobile Refinish Spray Coating Application (used in the Automobile Refinish Spray Coating operation)		

	Yderm = weight fraction of chemical in the liquid	
	FT = frequency of events (events/worker-day) (default: 1)	
Models for Calculating Worker De	rmal Exposures to a Solid Chemical	
EPA/OPPT Direct 2-Hand Dermal Contact with Solids Model	S x Qu = total amount of solids remaining on hands (mg/event)	Loading Solids into Transport Containers/Vessels (all activity types)
	(default: 3,100)	<u>Unloading</u> Solids from Transport Containers/Vessels (all activity types)
	Yderm = weight fraction of chemical in the liquid	<u>Cleaning</u> Solid Residuals from Transport Containers/Vessels (all activity types)
	FT = frequency of events	Sampling Solids (all activity type)
	(events/worker-day) (default: 1)	Equipment Cleaning Losses of Solids
		Filter Media Changeout
		Grinding and Sanding
		Miscellaneous Activities Related to Solids Processing
EPA/OPPT 2-Hand Contact with Container Surfaces Model	S x Qu = total amount of solids remaining on hands (mg/event) (default: 1,100)	There are no activities that use this model as a default for calculating worker dermal exposures to the chemical adhered to container surfaces.
	Yderm = weight fraction of chemical in the liquid	NOTE: It is recommended that you substitute this model for the default dermal model for any activity that would involve this type of worker contact.
	FT = frequency of events (events/worker-day) (default: 1)	
Models for Calculating Exposures	During Industry-Specific Activities	
Currently, there are no industry-sp	ecific activity dermal exposure models.	
Models for Calculating Exposures	During Other Generic Unit Operations	
User-Defined Dermal Model	S = surface area of contact (cm <sup>2</sup> ) (you	There are no activities that use this model as the default for calculating worker
	must choose or enter a value)	dermal exposures to the chemical.

(can be used to estimate dermal exposures to either a <u>liquid or</u> <u>solid</u> chemical)	Qu = quantity remaining on skin (mg/cm <sup>2</sup> -event) (you must choose or enter a value)	NOTE: You may substitute this model for the default dermal model for any activity for which you wish to enter an alternative known dermal surface area (S) and/or quantity remaining on the skin (Qu).
	Yderm = weight fraction of chemical in liquid	
	FT = frequency of events (events/worker-day) (default: 1)	

### List of OSHA PELS and NIOSH RELs

ChemSTEER includes various Occupational Safety and Health Administration (OSHA) Permissible Exposure Limits (PELs) and National Institute for Occupational Safety and Health (NIOSH) Recommended Exposure Limits (RELs) for more than 650 chemicals and other substances.

These PELs and RELs were obtained from the U.S. EPA's Endocrine Disruptor Priority Setting Database (EDPSD). These values were originally obtained from the following sources:

- NIOSH Pocket Guide (available on line at <a href="http://www.cdc.gov/niosh/npg/npg.html">http://www.cdc.gov/niosh/npg/npg.html</a>)
- Existing OSHA standards establishing PELs (available on line at: <u>http://www.osha.gov/SLTC/pel/index.html</u>)
- Additional exposure limits (i.e., STELs and CLs) documented in the 1988 OSHA Project Documentation website: <u>http://www.cdc.gov/niosh/pel88/pelstart.html</u>

To view ChemSTEER's set of PELs and RELs, click the *View Exposure Limits* button on the Chemical tab. The View OSHA PELs and NIOSH RELs window will appear. The selected Chemical Name, CAS Number, and Molecular Weight are displayed at the top of the window. There are also two subtabs: *PEL Information and REL Information*. In each of the subtabs, the PEL or REL information is displayed for the selected chemical. ChemSTEER's set of PELs and RELs incorporate at least one of the following values:

- Time-weighted average (TWA) PEL or REL concentration (Note: all TWAs are 8-hr averages, unless otherwise noted);
- PEL or REL short-term exposure limits (STELs); and
- PEL or REL ceiling (CL) exposure limits.

Each of the exposure limits are in units of mg/m<sup>3</sup> and parts-per-million (ppm). In many cases, the data source reported the limit in only one of these two units of measure. ERG used the chemical's molecular weight to convert the exposure limits into either mg/m<sup>3</sup> or ppm, as appropriate, using the following equations:

To convert an exposure limit concentration reported in mg/m3 into ppm:

To convert an exposure limit concentration reported in ppm into mg/m3:

Each of the PEL or REL values (i.e., TWAs, STELs, and CLs) includes an indicator of whether that value (ppm or mg/m3) was obtained by way of one of the above conversions. For example, Formaldehyde (CAS 50-00-0) has an OSHA 8-hr TWA PEL of 0.75 ppm. The PEL Information subtab

displays: "PEL TWA Converted (ppm? No". This indicates that the displayed TWA PEL of 0.75 ppm was taken directly from the source and was not the result of a conversion. Formaldehyde also includes a TWA PEL of 0.9212 mg/m3, with "PEL TWA Converted (mg/m3)? Yes". This indicates that the TWA PEL of 0.9212 mg/m3 was converted from the published ppm value using the equation above.

Some substances' PEL and/or REL limits could not be converted, as there is no molecular weight value for the substance (e.g., in the case of "wood dust" or "kaolin" exposure limits).

In addition, the set of exposure limits contains an OSHA TWA PEL concentration in units of millions of particles per cubic foot of air (mp/cfa) for the following substances:

- Mica (silicates):
- Talc (containing no asbestos fibers);
- Silica, amorphous, diatomaceous earth (uncalcined);
- Silica, amorphous, precipitated and gel; and
- Graphite.

The list also contains a NIOSH TWA REL for "fibrous glass" in units of fibers per cubic centimeter (f/cc).

#### Maneuvering the Set of PELs and RELs

Located at the bottom of each of the View OSHA PELs and NIOSH RELs window, the following buttons allow you to scroll through the set of PELs or RELs:

- Click either the *Next* > or < *Previous* buttons to move from one chemical record to another.
- Click the <<< *First* button to move directly to the first chemical record.
- Click the *Last* >>> button to move directly to the last chemical record.

You may search for a particular chemical record or filter the displayed set of chemical exposure limits by clicking the *New Search* button. Records can be filtered by either chemical name or CAS number. To return the full set of records, simply click the *New Search* button, leave the search field blank, and click *Search* to return to the exposure limit subtabs.

#### Models for Calculating Inhalation Exposures

#### EPA/OPPT Small Volume Solids Handling Inhalation Model

#### **Model Description**

This model utilizes worst case and typical exposure rates to estimate the amount of chemical inhaled by a worker during handling of "small volumes" (<54 kg/worker-shift) of solid/powdered materials containing the chemical. The handling of these small volumes is presumed to be scooping, weighing, and pouring of the solid materials.

#### Sources/Activities That Use This Model as a Default

The EPA/OPPT Small Volume Solids Handling Inhalation Model is the default for calculating worker inhalation exposures to a chemical while performing any source/activity for <u>Sampling Solids</u>.

#### **Other Sources/Activities**

The EPA/OPPT Small Volume Solids Handling Model may be an appropriate alternative to the default inhalation model for the following sources/activities:

#### Where the amount of material being handled is <u>less than</u> 54 kg/day:

- All sources/activities for <u>Cleaning Solid Residuals from Transport Containers/Vessels</u>
- All sources/activities for Loading Solids into Transport Containers/Vessels
- All sources/activities for <u>Unloading Solids from Transport Containers/Vessels</u>
- Equipment Cleaning Losses of Solids
- Miscellaneous Sources/Activities Related to Solid Processing

NOTE: If the amount of material being handled is unknown or was not calculated, the OSHA Total PNOR PEL-Limiting Model will be used as a default.

This model may be also used for the <u>Filter Media Changeout</u> source/activity, regardless of the amount of material.

#### Potential Route / Form(s) of Exposure

Inhalation / Particulate

#### Equations

Parameters	Description	Equation	Units
1	Inhalation potential dose rate	EF x AH x Ys x Sd	mg/day
NW	Total number of workers exposed	NWexp x NS	workers
LADD	Lifetime average daily dose	(I x ED x EY)/(BW x ATc x 365 days/yr)	mg/kg-day
ADD	Average daily dose	(I x ED x EY)/(BW x AT x 365 days/yr)	mg/kg-day
APDR	Acute potential dose rate	I/BW	mg/kg-day

#### **Model Input Parameters and Default Values**

The EPA/OPPT Small Volume Handling Inhalation Model default values for each of the input parameters are summarized in Table B-1.

Parameter	Description	Default Value(s)	Units
EF	Exposure Factor (mg exposure per kg solid handled)	Output 1: <u>Default:</u> 0.0477 (Typical) <u>Non-default :</u> 0.161 (Worst Case) Output 2: <u>Default:</u> 0.161 (Worst Case) <u>Non-default Option:</u> 0.0477 (Typical)	mg/kg
АН	The amount of solids/powder (containing the chemical ) handled ( $0 \le AH \le 54$ )	Defaults specified in Table B-1a	kg/worker- shift
Ys	Weight fraction of chemical in particulate $(0 \le Ys \le 1)$	Defaults specified in Table B-1b	dimensionless
Sd	Number of shifts worked by each worker during a workday ( $0 \le Sd \le 3$ )	1	shift/worker- day
NWexp	Number of workers exposed while performing the activity	1	worker/site
NS	Number of sites	NS (from Mass Balance Parameters subtab of the Operation Parameters tab)	site(s)
ED	Days exposed per year (0 ≤ ED (integer) ≤ 365)	Defaults specified in Table B-1c	days/site-yr
EY	Years of occupational exposure ( $0 \le EY$ )	40	years
BW	Body weight (0 ≤ BW)	70	kg
ATc	Averaging time over a lifetime (chronic) (0 ≤ ATc)	70	years
AT	Averaging time (EY $\leq$ AT $\leq$ ATc)	EY	years

## Table B-1. Input Parameters and Default Values for the EPA/OPPT Small Volume Handling Inhalation Model

You may elect to change any parameter from Table B-1 except EF, which is a constant. Clicking the *Type* column for each changeable parameter other than EF, AH, Ys, and ED contains only two options: ChemSTEER defaults from Table B-1 and User-defined. The conditional default and non-default options for AH, Ys, and ED are presented in the tables below. Be sure to read the <u>ChemSTEER Estimation</u> <u>Methods and Models</u> topic for more information about changing model parameters.

You may not change the defining model parameter, EF, to be anything other than one of the defaults shown above. If you wish to model inhalation exposures to solids using your own data, choose one of the following alternative models:

#### OSHA PEL-Limiting Model for Substance-Specific Particulates; or

User-Defined Inhalation Model.

NOTE: It is assumed that the same number of workers exposed by inhaling the chemical during the activity will also be dermally exposed (if a dermal exposure is expected). If you update the number of workers exposed (NWexp), the NWexp for the corresponding output in the dermal model, selected for the same activity, will be automatically updated with the entered value. For

example, if you update NWexp for Output 2 in this model, NWexp for Output 2 in the dermal model will be updated to the same value. The same is true if you update NWexp for Output 1.

#### Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Enabled* Enable Model Parameters for Output 2: *Enabled* 

Settings for either Output 1 or Output 2 results are based on which EF is selected for the corresponding output:

- Results using the typical exposure factor are characterized as *Typical* by default.
- Results using the worst case exposure factor are characterized as *Worst Case* by default.

You may select an alternative characterization for either of the outputs at any time.

#### **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Exposure Model Information* screen:

"EPA Small Volume Handling Model, less than 54 kg of PMN handled per site-day"

Source / Activity Type / Operation Mode	Batch Condition	Operation Type	Conditional AH Default* (kg/worker-shift)	Non-default Options for AH**
Container- Related / Continuous	Not Applicable	Any	MCi x Ncd (kg/site-day) (from Container Parameters subtab of the Operation Parameters tab)	DMIrm DMOprod User-defined AH
Container- Related / Batch	Any	Any	MCi x Ncd (kg/site-day) (from Container Parameters subtab of the Operation Parameters tab)	BMIrm BMOprod BMIrm x Ls (kg/site- bt) BMOprod x Ls (kg/site-bt) BMIrm x Nbd BMOprod x Nbd BMIrm x Nbd/Ls (kg/line-day) BMOprod x Nbd/Ls (kg/line-day) User-defined AH
Not Container- Related / Continuous	Not Applicable	Manufacturing	DMOprod (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMIrm User-defined AH
		Processing Use	DMIrm (kg/site-day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	DMOprod User-defined AH
Not Container- Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Manufacturing	BMOprod (kg/line-bt) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIrm BMIrm x Ls (kg/site- b t) BMOprod x Ls (kg/site-bt) User-defined AH
		Processing Use	BMIrm (kg/line-bt) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIprod BMIrm x Ls (kg/site- bt) BMOprod x Ls (kg/site-bt) User-defined AH
	Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of	Manufacturing	BMOprod x Nbd (kg/site- day) (from Mass Balance Parameters subtab of	BMIrm BMOprod BMIrm x Nbd BMIrm x Nbd/Ls

# Table B-1a. Conditional Default Values for AH for the EPA/OPPT Small Volume Handling Inhalation Model

the Operation Parameters tab)		the Operation Parameters tab)	(kg/line-day) BMOprod x Nbd/Ls (kg/line-day) User-defined AH
	Processing Use	BMIrm x Nbd (kg/site- day) (from Mass Balance Parameters subtab of the Operation Parameters tab)	BMIrm BMOprod BMOprod x Nbd BMIrm x Nbd/Ls (kg/line-day) BMOprod x Nbd/Ls (kg/line-day) User-defined AH

\* If the parameter or equation results in a default for AH > 54 kg/site-day, then ChemSTEER will display a pop-up warning and will not allow you to run the model until you select an option for which AH < 54 kg/site-day. \*\*Non-default options for AH are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab. All default and non-default options for AH are available for both Output 1 and Output 2.

**EPA Assessment Policy Recommendation:** It is recommended that, for solid residue cleaning activities, the amount of solid residue cleaned from or disposed with the emptied container, vessel, or process (i.e., the loss fraction x total amount in the container, vessel, or process) be used for AH in verifying the use of this model and in the calculations.

Source / Activity Type / Material Named in Source/Activity Label	Operation Type	Conditional Ys Default	Non-default Options for Ys*
Container-Related / Any	Any	Yi (from the Container Parameters subtabs of the Operation Parameters tab)	Yrm Yprod User-defined Ys
Not Container-Related / Raw Material	Any	Yrm (from the Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Ys
Not Container-Related / Product	Any	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Ys
Not Container-Related / Neither Raw Material nor Product	Manufacturing	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Ys
	Processing Use	Yrm (from the Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Ys

## Table B-1b. Conditional Default Values for Ys for the EPA/OPPT Small Volume Handling Inhalation Model

\*Non-default options for Ys are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab. All default and non-default options for Ys are available for both Output 1 and Output 2.

Source / Activity Type / Operation Mode	Batch Condition	Conditional ED Default (days of exposure/site-yr)	Non-default Options for ED*
Container-Related / Continuous or Batch	Any	Lesser of 250 or ODa (from Container Parameters subtab of the Operation Parameters tab)	Nby (bt/site-yr) OD (days/site- yr) User-defined ED
Not Container- Related / Continuous	Not Applicable	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	User-defined ED
Not Container- Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or Nby (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD User-defined ED
	Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby User-defined ED

## Table B-1c. Conditional Default Values for ED for the EPA/OPPT Small Volume Handling Inhalation Model

\*Non-default options for ED are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab. All default and non-default options for ED are available for both Output 1 and Output 2.

#### **Key Rationale for Model**

Worst case and typical exposure factor data (i.e., 0.161 mg/kg and 0.0477 mg/kg, respectively) were derived from a study of dye weighing and adapted for use in situations where workers are presumed to handle small volumes of solids in a manner similar to the handling in the study. The maximum amount of dye handled in the study was 54 kg per site-day. The exposure concentration is the same as the concentration of the chemical in the mixture.

#### References

US EPA/OPPT/CEB. Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991. (p. 4-11)

US EPA Chemical Engineering Branch Generic Scenario, Textile Dyeing, 10/15/92.

Textile Dye Weighing Monitoring Study. Exposure Evaluation Division, Economics and Technology Division, Office of Toxic Substances, U.S. Environmental Protection Agency, Washington, D.C. April 1990. EPA 560/5-90-009.

US EPA Memo entitled Draft Guidance on LADDs and APDRs from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93.

## EPA/OPPT Mass Balance Inhalation Model

#### **Model Description**

This model estimates the amount of chemical inhaled by a worker (typical and worst case) during an activity in which chemical vapor is generated. Estimation of the concentration for inhalation exposure is based on a vapor generation rate (G) estimated from a release model or from a user-input vapor generation rate. The following release models are vapor generation models:

<u>EPA/OAQPS AP-42 Loading Model</u> <u>EPA/OPPT Mass Transfer Coefficient Model</u> <u>EPA/OPPT Penetration Model</u> User-Defined Vapor Generation Rate Model

#### Sources/Activities That Use This Model as a Default

The EPA/OPPT Mass Balance Inhalation Model is the default for calculating worker inhalation exposures to a volatile chemical while performing the following sources/activities:

- All sources/activities involving <u>Cleaning Liquid Residuals from Transport</u> <u>Containers/Vessels</u>
- All sources/activities involving Loading Liquids into Transport Containers/Vessels
- All sources/activities involving <u>Unloading Liquids from Transport Containers/Vessels</u>
- All sources/activities involving <u>Sampling Liquids</u>
- Vapor Releases from Open Liquid Surfaces

NOTE: This model will be preselected for those activities in which the model is a default for calculating inhalation exposures; however, if the adjusted vapor pressure of the substance being handled (e.g., AVPrm, AVPprod) (calculated on the Operation Parameters tab, Shared Parameters/Factors subtab) is outside of the preferred range of adjusted vapor pressures (i.e., is less than AVPlow or greater than AVPhigh), then the model will not be selected. To read more about these settings, refer to the following topics:

- Vapor Model Activation
- <u>Operation Parameters Tab</u> → <u>Shared Parameters/Factors Subtab</u>

#### **Other Sources/Activities**

The EPA/OPPT Mass Balance Inhalation Model may be an appropriate alternative to the default inhalation model for the following sources/activities:

- All sources/activities for Equipment Cleaning Losses of Liquids
- Miscellaneous Sources/Activities Related to Liquid Processing
- Aqueous Wash of Organic Mass

- Distillation Column Bottoms Disposal
- Filter Media Changeout
- Liquid/Liquid Extraction Solvent Disposal
- <u>Scrubber Releases</u>

#### **Roll Coating**

#### Potential Route / Form(s) of Exposure

Inhalation / Vapor

#### Equations

Parameters	Description	Equation	Units
Cv	Volumetric concentration of chemical in air	Lesser of [(170,000 x T x G) / (MW x Q x k)] or [1,000,000 x X x VP / 760]	ppm
Cm	Mass concentration of chemical in air	Cv x MW / Vm	mg/m <sup>3</sup>
I	Inhalation potential dose rate	Cm x b x h	mg/day
NW	Total number of workers exposed	NWexp x NS	workers
LADD	Lifetime average daily dose	(I x ED x EY)/(BW x ATc x 365 days/yr)	mg/kg- day
ADD	Average daily dose	(I x ED x EY)/(BW x AT x 365 days/yr)	mg/kg- day
APDR	Acute potential dose rate	I/BW	mg/kg- day

#### **Model Input Parameters and Default Values**

The EPA/OPPT Mass Balance Inhalation Model default values for each of the input parameters are summarized in Table B-2.

Parameter	Description	Default Value(s)	Units
Т	Temperature of air (0 ≤ T)	298	К
G	Vapor generation rate	G (from the associated vapor generation model* or a User-defined G in the Release tab)	g/s
MW	Molecular weight of the chemical (0 ≤ MW)	MW (from chemical tab)	g/mol
Q	Ventilation rate (0 < Q)	Defaults specified in Table B-2a	ft³/min
k	Mixing factor ( $0 < k \le 1$ )	Defaults specified in Table B-2a	dimensionless
x	Vapor pressure correction factor (mole fraction or other) ( $0 \le X \le 1$ )	X (from the associated vapor generation model* or from the Shared Parameters/Factors subtab – Defaults specified in Table B-2b)	dimensionless
VP	Vapor pressure of the pure chemical being assessed (0 ≤ VP)	VP (from the associated vapor generation model* or VPchem from the Chemical tab)	torr
Vm	Molar volume (0 ≤ Vm)	24.45 @ 25°C, 1 atm	L/mol
b	Volumetric inhalation rate (0 < b ≤ 7.9)	1.25	m³/hr
h	Exposure duration (0 ≤ h ≤ 24)	Defaults specified in Table B-2c	hrs/day
ED	Days exposed per year (0 ≤ ED (integer) ≤ 365)	Defaults specified in Table B-2d	days/site-yr
NWexp	Number of workers exposed while performing the activity	1	workers/site
NS	Number of sites	NS (from Mass Balance Parameters subtab of the Operation Parameters tab)	site(s)
EY	Years of occupational exposure ( $0 \le EY$ )	40	years
BW	Body weight (0 ≤ BW)	70	kg
ATc	Averaging time over a lifetime (chronic) $(0 \le ATc)$	70	years
AT	Averaging time (EY ≤ AT ≤ ATc)	EY	years

Table B-2. In	put Parameters and	Default Values for	the FPA/OPPT	Mass Balance	Inhalation Model
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\*See Table B-2e for the hierarchy of logic for extracting *G*, *X*, and *VP* values from an associated release model.

You may elect to change any parameter from Table B-2. Clicking the *Type* column for each changeable parameter other than X and ED, contains only two options: ChemSTEER defaults from Table B-2 and User-defined. The default values of Q and k are dependent upon the selected source/activity and are summarized in Table B-2a. Similarly, the default value for h is dependent upon the selected source/activity, as summarized in Table B-2c. The conditional default and non-default options for X and ED are presented in Tables B-2b and B-2d, respectively. Be sure to read the <u>ChemSTEER Estimation</u> <u>Methods and Models</u> topic for more information about changing model parameters.

**NOTE:** It is assumed that the same number of workers exposed by inhaling the chemical during the activity will also be dermally exposed (if a dermal exposure is expected). If you update the number of workers exposed (NWexp), the NWexp for the corresponding output in the dermal model, selected for the same activity, will be automatically updated with the entered value. For example, if you update NWexp for Output 2 in this model, NWexp for Output 2 in the dermal model will be updated to the same value. The same is true if you update NWexp for Output 1.

#### Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Enabled* Enable Model Parameters for Output 2: *Enabled* 

Default Characterization of Output 1 Results: *Typical* Default Characterization of Output 2 Results: *Worst Case* 

NOTE: If you change the default value for either *Q* or *k*, the *Characterization of Results* will be automatically reset to Output 1 or Output 2 (as appropriate). You may select an alternative characterization for either of the outputs at any time.

#### **Default Model Basis**

The following default text is displayed in the Basis box on the View/Update Exposure Model Information screen:

"EPA/OPPT Mass Balance Model"

Vapor Generation Model Used for Source / Activity / Transport Container (if applicable)	Default Q <sup>1</sup> (cfm) (Characterization of Parameter Value)		Default k <sup>1</sup> (dimensionless) (Characterization of Parameter Value)	
	Output1	Output2	Output 1	Output 2
Outdoor Defaults: EPA/OAQPS AP-42 Loading Model / Rail Cars, Tank Trucks, or EPA/OPPT Mass Transfer Coefficient Model	237,600 (average)	26,400 x (60 x vz / 5280) <sup>3</sup> (worst case) (vz in ft/min; from associated vapor generation model on Releases tab)	0.5 (Typical)	0.1 (Worst Case)
Indoor Defaults: EPA/OAQPS AP-42 Loading Model / Transporting containers other than Rail Cars, Tan Trucks or EPA/OPPT Penetration Model or User-defined G or No vapor generation model used	3,000 (Typical)	500 (Worst Case)	0.5 (Typical)	0.1 (Worst Case)

#### Table B-2a. Conditional Default Values for k and Q for the EPA/OPPT Mass Balance Inhalation Model

Source: Chemical Engineering Branch Manual for the Preparation of Engineering Assessments (Tables 4-11 and 4-12)

1. Higher values for both parameters, Q and k, result in lower exposure estimates (i.e., as Output 1 results) based on the model equations.

2. The average default ventilation rate (Q) for outdoor activities is based upon an average wind speed of 9 mph (792 ft/min).

3. If the vapor generation model (e.g., EPA/OAQPS AP-42 Loading Model, etc.) does not use the parameter vz, ChemSTEER will use the default of 440 ft/min.

Associated Vapor Generation Model*	Material named in Source/Activity Label	Operation Type	Conditional X Default	Non-Default Options for X <sup>**</sup>
Yes	Any	Any	X (from associated vapor generation model* in the Releases tab)	Xrm Xprod Xother User- defined X
No <i>or</i> The associated vapor generation model does not contain an X value	Raw Material	Any	Xrm (from Shared Parameters/Factors subtab)	Xprod Xother User- defined X
	Product	Any	Xprod (from Shared Parameters/Factors subtab)	Xrm Xother User- defined X
	Other	Any	Xother (from Shared Parameters/Factors subtab)	Xrm Xother User- defined X
	Not material-specific	Manufacturing	Xprod (from Shared Parameters/Factors subtab)	Xrm Xother User- defined X
		Processing Use	Xrm (from Shared Parameters/Factors subtab)	Xprod Xother User- defined X

## Table B-2b. Conditional Default Values for X for the EPA/OPPT Mass Balance Inhalation Model

\*See Table B-2e for the hierarchy of logic for extracting an X value from an associated release model. \*\*Non-default options for X are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab. All default and non-default options for X are available for both Output 1 and Output 2.

Associated Release Model	Source / Activity Type	Conditional h Default* (hrs/site-day)
Yes	Any type	Lesser of 8 or OHa from an associated release model** (from Releases tab)
No	Container-Related	Lesser of 8 or OHa (from Container Parameters subtab of the Operation Parameters tab)
	Sampling	1
	Equipment Cleaning Losses of Liquids from Multiple Vessels	4
	Equipment Cleaning Losses of Liquids from a Single, Large Vessel	1
	Equipment Cleaning Losses of Liquids from a Single, Small Vessel	0.5
	Not Container-Related, Sampling, or Equipment Cleaning	8

#### Table B-2c. Conditional Default Values for h for the EPA/OPPT Mass Balance Inhalation Model

\*You may select the conditional default h (shown above) or enter a user-defined h for either Output 1 or Output 2 for all sources/activities. The conditional default h values were adopted as a policy decision in 2002. \*\*See Table B-2e for the hierarchy of logic for extracting an h value from an associated release model.

Associated Release Model / Source/Activity Type / Operation Mode	Batch Condition	Conditional ED Default (days of exposure/site-yr)	Non-default Options for ED**
Yes / Container-related / Continuous	Not applicable	Lesser of 250 or Freq from associated release model* (from Releases tab)	OD (days/site-yr) ODa (days/site-yr) User-defined ED
Yes / Container-related / Batch	Any	Lesser of 250 or Freq from associated release model* (from Releases tab)	Nby (bt/site-yr) OD (days/site-yr) ODa (days/site-yr) User-defined ED
Yes / Not Container-related / Continuous	Not applicable	Lesser of 250 or Freq from associated release model* (from Release tab)	OD (days/site-yr) User-defined ED
Yes / Not Container-related / Batch	Any	Lesser of 250 or Freq from associated release model* (from Releases tab)	Nby (bt/site-yr) OD (days/site-yr) User-defined ED
No associated release model / Container-Related / Continuous	Not applicable	Lesser of 250 or ODa (from Container Parameters subtab of the Operations Parameters tab)	OD (das/site-yr) User-defined ED
No associated release model /Container-Related /Batch	Any	Lesser of 250 or ODa (from Container Parameters subtab of the Operations Parameters tab)	Nby (bt/site-yr) OD (days/st-yr) User-defined ED
No associated release model	Not applicable	Lesser of 250 or OD	User-defined ED

#### Table B-2d. Conditional Default Values for ED for the EPA/OPPT Mass Balance Inhalation Model

/ Not Container-Related /Continuous		(from Mass Balance Parameters subtab of the Operation Parameters tab)	
No associated release model / Not Container-Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or Nby (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD (days/site-yr) User-defined ED
	Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby (bt/site-yr) User-defined ED

\*See Table B-2e for the hierarchy of logic for extracting an ED value from an associated release model. \*\*Non-default options for ED are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab. All default and non-default options for ED are available for both Output 1 and Output 2.

# Table B-2e. Hierarchy for Extracting Parameter Defaults from Associated Release Models\* for the EPA/OPPT Mass Balance Inhalation Model

- 1. Use current value of parameter from the last associated vapor generation model\* for the source/activity (from the *Releases* tab).
- 2. Use current value of parameter from the last associated release model\* for the source/activity (from the Releases tab) only if there is no associated vapor generation model.
- 3. If no associated release model\* for the source/activity, then use conditional default as described for "No associated release model" in Tables B-2b, and B-2c, and B-2d above.

\*The associated release model is the LAST vapor generation or release model that contains a parameter value required for the EPA/OPPT Mass Balance Inhalation Model that is listed in the *Release Model(s)* for *Selected Activity* box in the Releases tab (i.e., it is the last vapor generation or release model that was added by either ChemSTEER or the user) for the selected Source/Activity.

When extracting parameter values from the Releases tab, the *EPA/OPPT Mass Balance Model* Input Parameters for Output 1 are obtained from the associated release model Input Parameters for Output 1; and the *EPA/OPPT Mass Balance Model* Input Parameters for Output 2 are obtained from the associated release model Input Parameters for Output 2.

#### Key Rationale for Model

The airborne concentration of the chemical is estimated to be a function of the source vapor generation rate and the volumetric ventilation rate within a given space and includes simplifying assumptions of steady state (constant generation rate and constant ventilation rate) and a mixing factor (for non-ideal mixing of air). The default ventilation rates and mixing factors provide a typical and worst case estimate of exposure. The airborne concentration of the chemical cannot exceed the level of saturation for the chemical.

#### References
US EPA/OPPT/CEB. Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991. (Equations 4-1, 4-5, 4-14)

US EPA Memo entitled Draft Guidance on LADDs and APDRs from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93.

Fehrenbacher, M.C. and Hummel, A.A. "Evaluation of the Mass Balance Model Used by the Environmental Protection Agency for Estimating Inhalation Exposure to New Chemical Substances". American Industrial Hygiene Association Journal. June 1996. 57: 526-536.

# OSHA PEL-Limiting Model for Substance-Specific Particulates

## **Model Description**

This model estimates the amount of a chemical inhaled by a worker during handling of solid/powdered materials containing the chemical when the material/ mixture contains a specific substance with an OSHA Permissible Exposure Limit (PEL), Time-Weighted Average (TWA) or Ceiling (C). The estimate assumes that the worker is exposed to the chemical at a level limited by the OSHA PEL (TWA or C).

## Sources/Activities That Use This Model as a Default

The OSHA PEL-Limiting Model for Substance-Specific Particulates is the default for calculating worker inhalation exposures to a chemical contained in a mist while performing the <u>Operating the</u> <u>Electroplating Bath</u> activity.

NOTE: When used in this activity, the model uses the OSHA PEL for chromium (KCk=0.5 mg/m3) and an estimated chromium concentration in an electroplating bath (Ypel=0.25) as overriding defaults to those discussed below.

#### **Other Sources/Activities**

The OSHA PEL-Limiting Model for Substance-Specific Particulates may also be an appropriate means to calculate worker inhalation exposures to a solid, particulate chemical while performing the following sources/activities:

- All sources/activities for <u>Cleaning Solid Residuals from Transport Containers/Vessels</u>
- All sources/activities for Loading Solids into Transport Containers/Vessels
- All sources/activities for Unloading Solids from Transport Containers/Vessels
- All sources/activities for <u>Sampling Solids</u>

#### Coating Applications:

- Roll Coating
- Coating Using Hand Held Spray Gun

- Coating Using Hand Held Spray Can
- <u>Automobile OEM Spray Coating Application</u>
- <u>Automobile Refinish Spray Coating Application</u>

Other Sources/Activities:

- Equipment Cleaning Losses of Solids
- <u>Miscellaneous Sources/Activities Related to Liquid Processing Miscellaneous</u> Sources/Activities Related to Solid Processing

#### Potential Route / Form(s) of Exposure

Inhalation / Particulate or Mist

#### Equations

Parameters	Description	Equation	Units
Cm	Mass concentration of chemical in air	KCk x Ys / Ypel	mg/m <sup>3</sup>
I	Inhalation potential dose rate	Cm x b x h	mg/day
NW	Total number of workers exposed	NWexp x NS	workers
LADD	Lifetime average daily dose	(I x ED x EY)/(BW x ATc x 365 days/yr)	mg/kg-day
ADD	Average daily dose	(I x ED x EY)/(BW x AT x 365 days/yr)	mg/kg-day
APDR	Acute potential dose rate	I/BW	mg/kg-day

## **Model Input Parameters and Default Values**

The OSHA PEL-Limiting Model for Substance-Specific Particulates (TWA or C) default values for each of the input parameters are summarized in Table B-3.

Parameter	Description	Default Value(s)	Units
KCk	Mass concentration of the chemical or metal with a PEL in air (based on OSHA PEL – TWA)	15 (PNOR PEL)	mg/m <sup>3</sup>
Ys	Weight fraction of chemical in particulate (0 < Ys $\leq$ 1)*	Defaults specified in Table B-3a	dimensionless
Ypel	Weight fraction of chemical or metal with a PEL in particulate $(0 < Ypel \le 1)^*$	1	dimensionless
b	Volumetric inhalation rate ( $0 < b \le 7.9$ )	1.25	m³/hr
h	Exposure duration ( $0 \le h \le 24$ )	8	hrs/day
NWexp	Number of workers exposed while performing the activity	1	workers/site
NS	Number of sites	NS (from Mass Balance Parameters subtab of the Operation Parameters tab)	site(s)
ED	Days exposed per year (0 ≤ ED (integer) ≤ 365)	Defaults specified in Table B-3d	days/site-yr
EY	Years of occupational exposure ( $0 \le EY$ )	40	years
BW	Body weight (0 ≤ BW)	70	kg
ATc	Averaging time over a lifetime (chronic) (0 ≤ ATc)	70	years
AT	Averaging time (EY $\leq$ AT $\leq$ ATc)	EY	years

# Table B-3. Input Parameters and Default Values for the OSHA PEL-Limiting Model for Substance Specific Particulates (TWA or C)

\* Rather than using the specified weight fractions Ys and Ypel, you may also choose to enter relative mass values where Ys would be a relative weight of the chemical assessed and Ypel would be a relative weight of the substance with a PEL. For example, if in some total mixture there are 150 kg of chemical assessed for every 50 kg of substance with a PEL, any ratio of Ys: Ypel of 3 is valid. An option would be for you to enter 0.15 for Ys and 0.05 for Ypel. Another option would be for you to enter 0.3 for Ys and 0.1 for Ypel.

You may elect to change any parameter from Table B-3, except when h is a constant for a PEL that is based upon a specific TWA or C. The value of h may be changed when the PEL is a ceiling. Clicking the *Type* column for each changeable parameter other than Ys and ED contains only two options: ChemSTEER defaults from Table B-3 and User-defined. The conditional default and non-default options for Ys and ED are presented in the tables below. Be sure to read the <u>ChemSTEER Estimation Methods</u> and <u>Models</u> topic for more information about changing model parameters.

In future versions of ChemSTEER, non-default options for KCk will consist of a pick list of OSHA PELs for specific chemicals or metals from the Occupational Safety and Health Administration General Industry Air Contaminants Standard (29 CFR 1910.1000). In this version, you must determine and enter the appropriate value manually.

ChemSTEER contains a list of various OSHA PELS, as well as NIOSH Recommended Exposure Limits (RELs), for more than 700 chemicals and other substances. You may view this list by clicking on the *View/Update Exposure Limits* button, found on the Chemicals tab. To read more about this list, go to the <u>List of OSHA PELS and NIOSH RELs</u> topic. **NOTE:** It is assumed that the same number of workers exposed by inhaling the chemical during the activity will also be dermally exposed (if a dermal exposure is expected). If you update the number of workers exposed (NWexp), the NWexp for the corresponding output in the dermal model, selected for the same activity, will be automatically updated with the entered value. For example, if you update NWexp for Output 2 in this model, NWexp for Output 2 in the dermal model will be updated to the same value. The same is true if you update NWexp for Output 1.

### Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default Characterization of Output 1 Results: *Upper Bound* Default Characterization of Output 2 Results: *Upper Bound* 

You may select an alternative characterization for either of the outputs at any time.

## **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Exposure Model* Information screen:

"OSHA PEL-Limiting Model for Substance-specific Particulates (TWA or C)"

Table B-3a. Conditional Default Values for Ys for the OSHA PEL-Limiting Model for Substance-Specific
Particulates (TWA or C)

Source / Activity Type / Material Names in Source/Activity Type	Operation Type	Conditional Ys Default	Non-default Options for Ys*
Container-Related / Any	Any	Yi (from the Container Parameters subtabs of the Operation Parameters tab)	Yrm Yprod User-defined Ys
Not Container-Related / Raw Material	Any	Yrm (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Ys
Not Container-Related / Product	Any	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Ys
Not Container-Related /Neither Raw Material nor Product	Manufacturing	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Ys
	Processing Use	Yrm (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Ys

\*Non-default options for Ys are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab.

Source / Activity Type / Operation Mode	Batch Condition	Conditional ED Default (days of exposure/site-yr)	Non-default Options for ED*
Container-Related / Continuous	Not applicable	Lesser of 250 or ODa (from Container Parameters subtab of the Operation Parameters tab)	OD (days/site- yr) User-defined ED
Container-Related / Batch	Any	Lesser of 250 or ODa (from Container Parameters subtab of the Operation Parameters tab)	Nby (bt/site-yr) OD (days/site- yr) User-defined ED
Not Container- Related / Continuous	Not Applicable	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	User-defined ED
Not Container- Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or Nby (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD User-defined ED
	Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby User-defined ED

# Table B-3b. Conditional Default Values for ED for the OSHA PEL-Limiting Model for Substance-Specific Particulates (TWA or C)

\*Non-default options for ED are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab.

# Key Rationale for Model

Operations are generally expected to comply with OSHA's federal regulation regarding inhalation of specific chemicals. This model assumes that the exposure concentration of the chemical is at a ratio such that the concentration of the substance with a PEL is not exceeded.

# References

US EPA/OPPT/CEB. Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991. (Equations 4-1, 4-11)

US EPA Memo entitled Draft Guidance on LADDs and APDRs from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93.

# OSHA PEL-Limiting Model for Substance-Specific Vapors

Model Description

This model estimates the amount of vapor for a specific chemical inhaled by a worker during handling of liquid material containing the chemical when the mixture contains a chemical with an OSHA Permissible Exposure Limit (PEL), Time-Weighted Average (TWA) or Ceiling (C), or when controls are in place that would limit exposure of a chemical with an OSHA PEL. The estimate assumes that the worker is exposed to the chemical with a PEL at a level no greater than the OSHA PEL (TWA or C).

Some of the default input parameter values used by this model are derived from an associated release model used to estimate releases of vapors during the activity. The following release models may provide the default values for some input parameters:

EPA/OAQPS AP-42 Loading Model EPA/OPPT Mass Transfer Coefficient Model EPA/OPPT Penetration Model User-Defined Vapor Generation Rate Model

#### Sources/Activities That Use This Model as a Default

There are no sources/activities in ChemSTEER that use this model as a default for calculating worker inhalation exposures to a chemical.

## **Other Sources/Activities**

The OSHA PEL-Limiting Model for Substance-Specific Vapors may be an appropriate means to calculate worker exposures to a volatile chemical while performing the following sources/activities:

- All sources/activities for Cleaning Liquid Residuals from Transport Containers/Vessels
- All sources/activities for Equipment Cleaning Losses of Liquids
- All sources/activities for Loading Liquids into Transport Containers/Vessels
- All sources/activities for Unloading Liquids from Transport Containers/Vessels
- All <u>Generic Coating Applications</u> sources/activities
- All <u>Automobile Spray Coating</u> sources/activities
- <u>Miscellaneous Sources/Activities Related to Liquid Processing</u>
- Vapor Releases from Open Liquid Surfaces

Unit Operations and Processes:

- Aqueous Wash of Organic Mass
- Distillation Column Bottoms Disposal
- Filter Media Changeout
- Liquid/Liquid Extraction Solvent Disposal
- <u>Scrubber Releases</u>

# **Potential Exposure Route**

Inhalation / Vapor

## Equations

Parameters	Description	Equation	Units
Cvk	Volumetric concentration of chemical in air	Lesser of [(Cvk x (VP x Ys / MW) / (VPpel x Ypel / MWpel)]	ppm
		or [1,000,000 x X x VP/ 760]	
Cm	Mass concentration of chemical in air	Cv x MW / Vm	mg/m <sup>3</sup>
I	Inhalation potential dose rate	Cm x b x h	mg/day
NW	Total number of workers exposed	NWexp x NS	workers
LADD	Lifetime average daily dose	(I x ED x EY)/(BW x ATc x 365 days/yr)	mg/kg- day
ADD	Average daily dose	(I x ED x EY)/(BW x AT x 365 days/yr)	mg/kg- day
APDR	Acute potential dose rate	I/BW	mg/kg- day

## **Model Input Parameters and Default Values**

The OSHA PEL-Limiting Model for Substance-Specific Vapor (TWA or C) default values for each of the input parameters are summarized in Table B-4.

Parameter	Description	Default Value(s)	Units
Cvk	Vapor concentration of the chemical with a PEL in air (based on OSHA PEL – TWA)	User-defined Cvk <sup>1</sup>	ppm
VP	Vapor pressure of the pure chemical being assessed (0 ≤ VP)	VP (from the associated vapor generation model <sup>2</sup> or VPchem in the Chemical tab)	torr
Ys	Weight fraction of the chemical in mixture <sup>3</sup>	Defaults specified in Table B-4a	dimensionless
MW	Molecular weight of the chemical (0 ≤ MW)	MW (from Chemical tab)	g/mol
VPpel	Vapor pressure of the pure PEL chemical	User-defined VPpel <sup>1</sup>	torr
Ypel	Weight fraction of chemical with PEL in mixture <sup>3</sup>	1 – Ys	dimensionless
MWpel	Molecular weight of the PEL chemical	User-defined MWpel <sup>1</sup>	g/mol
x	Vapor pressure correction factor (mole fraction or other $(0 \le X \le 1)$	X (from the associated vapor generation model <sup>2</sup> or from the Shared Parameters/Factors subtab – Defaults specified in Table 19-b)	dimensionless
Vm	Molar volume (0 ≤ Vm)	24.45 @ 25°C, 1 atm	L/mol
b	Volumetric inhalation rate (0 < b ≤ 7.9)	1.25	m³/hr
h	Exposure duration (0 ≤ h ≤ 24)	8	hrs/day
NWexp	Number of workers exposed while performing the activity	1	workers/site
NS	Number or sites	NS (from Mass Balance Parameters subtab of the Operation Parameters tab)	site(s)
ED	Days exposed per year (0 ≤ ED (integer) ≤ 365)	Defaults specified in Table B-4c	days/site-yr
EY	Years of occupational exposure (0 ≤ EY)	40	years
BW	Body weight (0 ≤ ATc)	70	kg
ATc	Averaging time over a lifetime (chronic) (0 ≤ ATc)	70	years
AT	Averaging time (EY ≤ AT ≤ ATc)	EY	years

# Table B-4. Input Parameters and Default Values for the OSHA PEL-Limiting Model for Substance-Specific Vapor (TWA or C)

1. You must select and manually input values of the OSHA PEL for the appropriate chemical, its molecular weight, and its vapor pressure. In future versions of ChemSTEER, the user will choose a chemical from a pick list of OSHA PEL chemicals from the Occupational Safety and Health Administration General Industry Air Contaminants Standard (29 CFR 1910.1000.), and ChemSTEER will automatically retrieve the Cvk, molecular weight, and vapor pressure for the PEL chemical. ChemSTEER contains a list of various OSHA PELS, as well as NIOSH Recommended Exposure Limits (RELs), for more than 700 chemicals and other substances. You may view this list by clicking on the *View/Update Exposure Limits* button, found on the *Chemicals* tab. To read more about this list, go to the <u>List of OSHA PELS and NIOSH RELs</u> topic.

2. See Table B-4d for the hierarchy of logic for extracting VP, X, and ED values from an associated release model. 3. Rather than using the specified weight fractions Ys and Ypel, you may also choose to enter relative mass values where Ys would be a relative weight of the chemical assessed and Ypel would be a relative weight of the substance with a PEL. For example, if in some total mixture there are 150 kg of chemical assessed for every 50 kg of substance with a PEL, any ratio of Ys: Ypel of 3 is valid. An option would be for you to enter 0.15 for Ys and 0.05 for Ypel. Another option would be for you to enter 0.3 for Ys and 0.1 for Ypel.

You may elect to change any parameter from Table B-4, except when h is a constant for a PEL that is based upon a specific TWA. The value of h may be changed when the PEL is a ceiling. Clicking the *Type* column for each changeable parameter other than Cvk, Ys, VPpel, MWpel, X, and ED contains only two options: ChemSTEER defaults from Table B-4 and User-defined. You <u>must</u> enter values for Cvk, VPpel, and MWpel in this exposure model. The conditional default and non-default options for Ys, X, and ED are presented in the tables below. Be sure to read the <u>ChemSTEER Estimation Methods and Models</u> topic for more information about changing model parameters.

NOTE: It is assumed that the same number of workers exposed by inhaling the chemical during the activity will also be dermally exposed (if a dermal exposure is expected). If you update the number of workers exposed (NWexp), the NWexp for the corresponding output in the dermal model, selected for the same activity, will be automatically updated with the entered value. For example, if you update NWexp for Output 2 in this model, NWexp for Output 2 in the dermal model will be updated to the same value. The same is true if you update NWexp for Output 1.

#### Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* Default Characterization of Output 1 Results: *Upper Bound* Default Characterization of Output 2 Results: *Upper Bound* 

You may select an alternative characterization for either of the outputs at any time.

#### **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Exposure Model Information* screen:

"OSHA PEL-Limiting Model for Substance-Specific Vapor (TWA or C)"

Source / Activity Type / Material Names in Source/Activity Type	Operation Type	Conditional Ys Default	Non-default Options for Ys*
Container-Related / Any	Any	Yi (from the Container Parameters subtabs of the Operation Parameters tab)	Yrm Yprod User-defined Ys
Not Container-Related / Raw Material	Any	Yrm (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Ys
Not Container-Related / Product	Any	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Ys
Not Container-Related /Neither Raw Material nor Product	Manufacturing	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Ys
	Processing Use	Yrm (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Ys

# Table B-4a. Conditional Default Values for Ys for the OSHA PEL-Limiting Model for Substance-Specific Vapor (TWA or C)

\*Non-default options for Ys are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab.

Associated Vapor Generation Model*	Material named in Source/Activity Label	Operation Type	Conditional X Default	Non-Default Options for X**
Yes	Any	Any	X (from associated vapor generation model* in the Releases tab)	Xrm Xprod Xother User- defined X
No <i>or</i> The associated vapor generation model does not contain an X value	Raw Material	Any	Xrm (from Shared Parameters/Factors subtab)	Xprod Xother User- defined X
	Product	Any	Xprod (from Shared Parameters/Factors subtab)	Xrm Xother User- defined X
	Other	Any	Xother (from Shared Parameters/Factors subtab)	Xrm Xother User- defined X
	Not material-specific	Manufacturing	Xprod (from Shared Parameters/Factors subtab)	Xrm Xother User- defined X
		Processing Use	Xrm (from Shared Parameters/Factors subtab)	Xprod Xother User- defined X

# Table B-4b. Conditional Default Values for X for the OSHA PEL-Limiting Model for Substance-SpecificVapor (TWA or C)

\*See Table B-4d for the hierarchy of logic for extracting an X value from an associated release model. \*\*Non-default options for X are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab.

Associated Release Model / Source/Activity Type / Operation Mode	Batch Condition	Conditional ED Default (days of exposure/site-yr)	Non-default Options for ED**
Yes / Container-related / Continuous	Not applicable	Lesser of 250 or Freq from associated release model* (from Releases tab)	OD (days/site- yr) ODa (days/site- yr) User-defined ED
Yes / Container-related / Batch	Any	Lesser of 250 or Freq from associated release model* (from Releases tab)	Nby (bt/site-yr) OD (days/site- yr) ODa (days/site- yr) User-defined ED
Yes / Not Container-related / Continuous	Not applicable	Lesser of 250 or Freq from associated release model* (from Release tab)	OD (days/site- yr) User-defined ED
Yes / Not Container-related / Batch	Any	Lesser of 250 or Freq from associated release model* (from Releases tab)	Nby (bt/site-yr) OD (days/site- yr) User-defined ED
No associated release model / Container-Related / Continuous	Not applicable	Lesser of 250 or ODa (from Container Parameters subtab of the Operations Parameters tab)	OD (das/site-yr) User-defined ED
No associated release model /Container-Related /Batch	Any	Lesser of 250 or ODa (from Container Parameters subtab of the Operations Parameters tab)	Nby (bt/site-yr) OD (days/st-yr) User-defined ED
No associated release model / Not Container-Related /Continuous	Not applicable	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	User-defined ED
No associated release model / Not Container-Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or Nby (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD (days/site- yr) User-defined ED
	Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby (bt/site-yr) User-defined ED

# Table B-4c. Conditional Default Values for ED for the OSHA PEL-Limiting Model for Substance-SpecificVapor (TWA or C)

\*See Table B-4d for the hierarchy of logic for extracting an ED value from an associated release model. \*\*Non-default options for ED are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab.

# Table B-4d. Hierarchy for Extracting Parameter Defaults from Associated Release Models\* for the OSHA PEL-Limiting Model for Substance-Specific Vapor (TWA or C)

- 1. Use current value of parameter from the last associated vapor generation model\* for the source/activity (from the *Releases* tab).
- 2. Use current value of parameter from the last associated release model\* for the source/activity (from the Releases tab) only if there is no associated vapor generation model.
- 3. If no associated release model\* for the source/activity, then use conditional default as described for "No associated release model" in Tables B-4, and B-4b, and B-4c above.

\*The associated *release model* is the LAST vapor generation or release model that contains a parameter value required for the OSHA PEL-Limiting Model for Substance Specific Vapor that is listed in the *Release Model(s)* for *Selected Activity* box in the Releases tab (i.e., it is the last vapor generation or release model that was added by either ChemSTEER or the user) for the selected Source/Activity.

When extracting parameter values from the Releases tab, the OSHA PEL-Limiting Model for Substance-Specific Vapors Input Parameters for Output 1 are obtained from the associated release model Input Parameters for Output 1; and the OSHA PEL-Limiting Model for Substance-Specific Vapors Input Parameters for Output 2 are obtained from the associated release model Input Parameters for Output 2 are obtained from the associated release model Input Parameters for Output 2.

# Key Rationale for Model

Operations are generally expected to comply with OSHA's federal regulation regarding inhalation of specific chemicals. This model assumes that the exposure concentration of the chemical is at a ratio such that the concentration of the substance with a PEL is not exceeded.

#### References

US EPA/OPPT/CEB. Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991. (Equations 4-1, 4-4)

US EPA Memo entitled Draft Guidance on LADDs and APDRs from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93.

# OSHA Total PNOR PEL-Limiting Model

#### **Model Description**

This model estimates the amount of chemical inhaled by a worker during handling of solid/ powdered materials containing the chemical. The estimate assumes that the worker is exposed at a level no greater than the OSHA Permissible Exposure Limit (PEL) for Particulate, Not Otherwise Regulated (PNOR), total particulate.

### Sources/Activities That Use This Model as a Default

The OSHA Total PNOR PEL-Limiting Model is the default for calculating worker inhalation exposures to a chemical while performing the following sources/activities:

- Grinding and Sanding
- Coating Using Hand Held Spray Gun

## **Other Sources/Activities**

The OSHA Total PNOR PEL-Limiting Model may be an appropriate alternative to the default inhalation model for the following sources/activities:

*Where the amount of material being handled is <u>more than</u> 54 kg/day (or where the amount of material is unknown or was not previously calculated):* 

- All sources/activities for <u>Cleaning Solid Residuals from Transport Containers/Vessels</u>
- All sources/activities for Loading Solids into Transport Containers/Vessels
- All sources/activities for Vessels
- Equipment Cleaning Losses of Solids
- Miscellaneous Sources/Activities Related to Solid Processing

This model may be also used for the following sources/activities, regardless of the amount of material:

- All sources/activities for <u>Sampling Solids</u>
- <u>Miscellaneous Sources/Activities Related to Liquid Processing</u>
- Filter Media Changeout
- Roll Coating

#### Potential Route / Form(s) of Exposure

Inhalation / Particulate or non-volatile portion of mist, aerosols, etc.

#### Equations

Parameters	Description	Equation	Units
Cm	Mass concentration of chemical in air	KCk x Ys	mg/m <sup>3</sup>
I	Inhalation potential dose rate	Cm x b x h	mg/day
NW	Total number of workers exposed	NWexp x NS	workers
LADD	Lifetime average daily dose	(I x ED x EY)/(BW x ATc x 365 days/yr)	mg/kg-day
ADD	Average daily dose	(I x ED x EY)/(BW x AT x 365 days/yr)	mg/kg-day
APDR	Acute potential dose rate	I/BW	mg/kg-day

### **Model Input Parameters and Default Values**

The OSHA Total PNOR PEL-Limiting Model default values for each of the input parameters are summarized in Table B-5.

Parameter	Description	Default Value(s)	Units
KCk	Mass concentration of total particulate in air (based on OSHA PEL for PNOR – TWA)	15	mg/ m <sup>3</sup>
Ys	Weight fraction of the chemical in particulate (or in solids portion of mist, etc.) (0 ≤ Ys ≤ 1)	Defaults specified in Table B-5a	dimensionless
b	Volumetric inhalation rate ( $0 < b \le 7.9$ )	1.25	m³/hr
h	Exposure duration ( $0 \le h \le 24$ )	8	hrs/day
NWexp	Number of workers exposed while performing the activity	1	workers/site
NS	Number or sites	NS (from Mass Balance Parameters subtab of the Operation Parameters tab)	site(s)
ED	Days exposed per year (0 ≤ ED (integer) ≤ 365)	Defaults specified in Table B-5c	days/site-yr
EY	Years of occupational exposure ( $0 \le EY$ )	40	years
BW	Body weight ( $0 \le ATc$ )	70	kg
ATc	Averaging time over a lifetime (chronic) (0 ≤ ATc)	70	years
AT	Averaging time (EY ≤ AT ≤ ATc)	EY	years

Table B-5. Input Parameters a	nd Default Values for the OSHA	<b>Total PNOR PEL-Limiting Model</b>
· · · · · · · · · · · · · · · · · · ·		

You may elect to change any parameter from Table B-5 except KCk and h, which are constants. Clicking the *Type* column for each changeable parameter other than KCk, h, Ys and ED contains only two options: ChemSTEER defaults from Table B-5 and User-defined. The conditional default and non-default options for Ys and ED are presented in the tables below. Be sure to read the <u>ChemSTEER Estimation</u> <u>Methods and Models</u> topic for more information about changing model parameters.

You may not change the defining model parameters, KCk and h, to be anything other than the defaults shown above. If you wish to model inhalation exposures to solids using your own PEL data, choose the OSHA PEL-Limiting Model for Substance-Specific Particulates.

**NOTE:** It is assumed that the same number of workers exposed by inhaling the chemical during the activity will also be dermally exposed (if a dermal exposure is expected). If you update the number of workers exposed (NWexp), the NWexp for the corresponding output in the dermal model, selected for the same activity, will be automatically updated with the entered value. For example, if you update NWexp for Output 2 in this model, NWexp for Output 2 in the dermal model will be updated to the same value. The same is true if you update NWexp for Output 1.

#### Default Parameter Value Switch Settings and Results Characterization:

Enable Model Parameters for Output 1: Disabled

Enable Model Parameters for Output 2: Enabled

Default Characterization of Output 1 Results: *Upper Bound* Default Characterization of Output 2 Results: *Upper Bound* 

You may select an alternative characterization for either of the outputs at any time.

## **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Exposure Model Information* screen:

"OSHA PNOR PEL-Limiting Model"

#### Table B-5a. Conditional Default Values for Ys for the OSHA Total PNOR PEL-Limiting Model

Source / Activity Type / Material Names in Source/Activity Type	Operation Type	Conditional Ys Default	Non-default Options for Ys*	
Sources/Activities Handling Solids				
Container-Related / Any	Any	Yi (from the Container Parameters subtabs of the Operation Parameters tab)	Yrm Yprod User-defined Ys	
Not Container-Related / Raw Material	Any	Yrm (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Ys	
Not Container-Related / Product	Any	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Ys	
Not Container-Related /Neither Raw Material nor Product	Manufacturing	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Ys	
	Processing Use	Yrm (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Ys	
Sources/Activities Handling Liquids and Unspecified Materials				
Container-Related / Any	Not applicable	User-defined Ys	Yi Yrm Yprod	
Not Container-Related / Any	Not applicable	User-defined Ys	Yrm Yprod	

\*Non-default options for Ys are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab.

Source / Activity Type / Operation Mode	Batch Condition	Conditional ED Default (days of exposure/site-yr)	Non-default Options for ED*
Container-Related / Continuous	Not applicable	Lesser of 250 or ODa (from Container Parameters subtab of the Operation Parameters tab)	OD (days/site- yr) User-defined ED
Container-Related / Batch	Any	Lesser of 250 or ODa (from Container Parameters subtab of the Operation Parameters tab)	Nby (bt/site-yr) OD (days/site- yr) User-defined ED
Not Container- Related / Continuous	Not Applicable	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	User-defined ED
Not Container- Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or Nby (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD User-defined ED
	Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby User-defined ED

# Table B-5b. Conditional Default Values for ED for the OSHA Total PNOR PEL-Limiting Model

\*Non-default options for ED are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab.

#### Key Rationale for Model

Operations are generally expected to comply with OSHA's federal regulation regarding total particulate exposures. This model assumes that the exposure concentration is the same as the concentration of the chemical in the mixture.

#### References

US EPA/OPPT/CEB. Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991. (Equations 4-1, 4-11)

US EPA Memo entitled Draft Guidance on LADDs and APDRs from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93.

#### OSHA Respirable PNOR PEL-Limiting Model

#### **Model Description**

This model estimates the amount of chemical inhaled by a worker during handling of solid/ powdered materials containing the chemical. The estimate assumes that the worker is exposed at a level

no greater than the OSHA Permissible Exposure Limit (PEL) for Particulate, Not Otherwise Regulated (PNOR), respirable particulate.

#### Sources/Activities That Use This Model as a Default

There are no sources/activities in ChemSTEER that use this model as a default for calculating worker inhalation exposures to a chemical.

### **Other Sources/Activities**

The OSHA Respirable PNOR PEL-Limiting Model may also be an appropriate means to calculate worker inhalation exposures to a solid, particulate chemical while performing the following sources/activities:

- All sources/activities for <u>Cleaning Solid Residuals from Transport Containers/Vessels</u>
- All sources/activities for Loading Solids into Transport Containers/Vessels
- All sources/activities for Unloading Solids from Transport Containers/Vessels
- All sources/activities for <u>Sampling Solids</u>
- Equipment Cleaning Losses of Solids
- Miscellaneous Sources/Activities Related to Liquid Processing
- Miscellaneous Sources/Activities Related to Solid Processing
- Filter Media Changeout
- Grinding and Sanding
- Roll Coating

# Potential Route / Form(s) of Exposure

Inhalation / Particulate or non-volatile portion of mist, aerosols, etc.

#### Equations

Parameters	Description	Equation	Units
Cm	Mass concentration of chemical in air	KCk x Ys	mg/m <sup>3</sup>
1	Inhalation potential dose rate	Cm x b x h	mg/day
NW	Total number of workers exposed	NWexp x NS	workers
LADD	Lifetime average daily dose	(I x ED x EY)/(BW x ATc x 365 days/yr)	mg/kg-day
ADD	Average daily dose	(I x ED x EY)/(BW x AT x 365 days/yr)	mg/kg-day
APDR	Acute potential dose rate	I/BW	mg/kg-day

# **Model Input Parameters and Default Values**

The OSHA Respirable PNOR PEL-Limiting Model default values for each of the input parameters are summarized in Table B-6.

Parameter	Description	Default Value(s)	Units
KCk	Mass concentration of total particulate in air (based on OSHA PEL for PNOR – TWA)	5	mg/ m <sup>3</sup>
Ys	Weight fraction of the chemical in particulate (or in solids portion of mist, etc.) (0 ≤ Ys ≤ 1)	Defaults specified in Table B-6a	dimensionless
b	Volumetric inhalation rate ( $0 < b \le 7.9$ )	1.25	m³/hr
h	Exposure duration ( $0 \le h \le 24$ )	8	hrs/day
NWexp	Number of workers exposed while performing the activity	1	workers/site
NS	Number or sites	NS (from Mass Balance Parameters subtab of the Operation Parameters tab)	site(s)
ED	Days exposed per year (0 ≤ ED (integer) ≤ 365)	Defaults specified in Table B-4c	days/site-yr
EY	Years of occupational exposure ( $0 \le EY$ )	40	years
BW	Body weight (0 ≤ ATc)	70	kg
ATc	Averaging time over a lifetime (chronic) (0 ≤ ATc)	70	years
AT	Averaging time (EY $\leq$ AT $\leq$ ATc)	EY	years

#### Table B-6. Input Parameters and Default Values for the OSHA Respirable PNOR PEL-Limiting Model

You may elect to change any parameter from Table B-6 except KCk and h, which are constants. Clicking the *Type* column for each changeable parameter other than KCk, h, Ys and ED contains only two options: ChemSTEER defaults from Table B-6 and User-defined. The conditional default and non-default options for Ys and ED are presented in the tables below. Be sure to read the <u>ChemSTEER Estimation</u> <u>Methods and Models</u> topic for more information about changing model parameters.

You may not change the defining model parameters, KCk and h, to be anything other than the defaults shown above. If you wish to model inhalation exposures to solids using your own PEL data, choose the OSHA PEL-Limiting Model for Substance-Specific Particulates.

NOTE: It is assumed that the same number of workers exposed by inhaling the chemical during the activity will also be dermally exposed (if a dermal exposure is expected). If you update the number of workers exposed (NWexp), the NWexp for the corresponding output in the dermal model, selected for the same activity, will be automatically updated with the entered value. For example, if you update NWexp for Output 2 in this model, NWexp for Output 2 in the dermal model will be updated to the same value. The same is true if you update NWexp for Output 1.

#### Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default Characterization of Output 1 Results: *Upper Bound* Default Characterization of Output 2 Results: *Upper Bound*  You may select an alternative characterization for either of the outputs at any time.

### **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Exposure Model Information* screen:

"OSHA Respirable PNOR PEL-Limiting Model"

## Table B-6a. Conditional Default Values for Ys for the OSHA Respirable PNOR PEL-Limiting Model

Source / Activity Type / Material Names in Source/Activity Type	Operation Type	Conditional Ys Default	Non-default Options for Ys*		
Sources/Activities Handling Solids					
Container-Related / Any	Any	Yi (from the Container Parameters subtabs of the Operation Parameters tab)	Yrm Yprod User-defined Ys		
Not Container-Related / Raw Material	Any	Yrm (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Ys		
Not Container-Related / Product	Any	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Ys		
Not Container-Related /Neither Raw Material nor Product	Manufacturing	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Ys		
	Processing Use	Yrm (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Ys		
Sources/Activities Handling Liquids a	nd Unspecified Ma	aterials			
Container-Related / Any	Not applicable	User-defined Ys	Yi Yrm Yprod		
Not Container-Related / Any	Not applicable	User-defined Ys	Yrm Yprod		

\*Non-default options for Ys are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab.

Source / Activity Type / Operation Mode	Batch Condition	Conditional ED Default (days of exposure/site-yr)	Non-default Options for ED*
Container-Related / Continuous	Not applicable	Lesser of 250 or ODa (from Container Parameters subtab of the Operation Parameters tab)	OD (days/site- yr) User-defined ED
Container-Related / Batch	Any	Lesser of 250 or ODa (from Container Parameters subtab of the Operation Parameters tab)	Nby (bt/site-yr) OD (days/site- yr) User-defined ED
Not Container- Related / Continuous	Not Applicable	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	User-defined ED
Not Container- Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or Nby (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD User-defined ED
	Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby User-defined ED

Table B-6b.	Conditional De	efault Values for	ED for the OS	SHA Respirable I	PNOR PEL-Limiting	g Model
						J

\*Non-default options for ED are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab.

#### **Key Rationale for Model**

Operations are generally expected to comply with OSHA's federal regulation regarding respirable particulate exposures. This model assumes that the exposure concentration is the same as the concentration of the chemical in the mixture.

#### References

US EPA/OPPT/CEB. Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991. (Equations 4-1, 4-11)

US EPA Memo entitled Draft Guidance on LADDs and APDRs from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93.

# EPA/OPPT Automobile OEM Spray Coating Inhalation Exposure Model

#### **Model Description**

This model estimates the amount of non-volatile non-polyisocyanate chemical in mist inhaled by a worker spray painting automobiles in automobile OEM coating operations. This model uses mist concentration data based upon spray gun type and booth type.

## Sources/Activities That Use This Model as a Default

The EPA/OPPT Automobile OEM Spray Coating Inhalation Exposure Model (non-volatile, non-polyisocyanates) is the default for calculating worker exposures to a non-volatile, non-polyisocyanate chemical during the <u>Automobile OEM Spray Coating Application</u> source/activity.

This model is not used as an alternative inhalation exposure model for any other sources/activities.

## Potential Route / Form(s) of Exposure

Inhalation / Particulate or non-volatile portion of mist, aerosols, etc.

#### Equations

Parameters	Description	Equation	Units
Cm	Mass concentration of chemical in air	KCk x Ys	mg/m <sup>3</sup>
I	Inhalation potential dose rate	Cm x b x h	mg/day
NW	Total number of workers exposed	NWexp x NS	workers
LADD	Lifetime average daily dose	(I x ED x EY)/(BW x ATc x 365 days/yr)	mg/kg-day
ADD	Average daily dose	(I x ED x EY)/(BW x AT x 365 days/yr)	mg/kg-day
APDR	Acute potential dose rate	I/BW	mg/kg-day

#### **Model Input Parameters and Default Values**

The EPA/OPPT Automobile OEM Spray Coating Inhalation Exposure Model default values for each of the input parameters are summarized in Table B-7.

Parameter	Description	Default Value(s)	Units
KCk	Mass concentration of total particulate in air	Non-default options specified in Table B-7a	mg/ m <sup>3</sup>
Ys	Weight fraction of the chemical in particulate or solids fraction of mist ( $0 \le Ys \le 1$ )	Lesser of (Ymist/Ysf) or 1 or User-defined Ys	dimensionless
Ymist	Weight fraction of chemical in mist (0 ≤ Ymist ≤ 1)	Non-default options specified in Table B-7b	dimensionless
Ysf	Weight fraction of solids in paint ( $0 \le Ysf \le 1$ )	0.25*	dimensionless
b	Volumetric inhalation rate ( $0 < b \le 7.9$ )	1.25	m³/hr
h	Exposure duration ( $0 \le h \le 24$ )	8	hrs/day
NWexp	Number of workers exposed while performing the activity	17	workers/site
NS	Number or sites	NS (from Mass Balance Parameters subtab of the Operation Parameters tab)	site(s)
ED	Days exposed per year (0 ≤ ED (integer) ≤ 365)	Defaults specified in Table B-7c	days/site-yr
EY	Years of occupational exposure ( $0 \le EY$ )	40	years
BW	Body weight (0 ≤ ATc)	70	kg
ATc	Averaging time over a lifetime (chronic) (0 ≤ ATc)	70	years
AT	Averaging time (EY $\leq$ AT $\leq$ ATc)	EY	years

# Table B-7. Input Parameters and Default Values for the EPA/OPPT Automobile OEM Spray Coating Inhalation Exposure Model (non-volatile non-polyisocyanates)

\*The reference generic scenario suggests a default solids fraction of 0.25. It also states that "'high solids paint' for automobiles can have a solids content of up to 45 to 50 volume percent to top coats...; however, solids content varies widely."

You may elect to change any parameter from Table B-7. If you input a user-defined value for Ys, the values of Ymist and Ysf are not used in the model. Clicking the *Type* column for each changeable parameter other than KCk, Ymist, and ED contains only two options: ChemSTEER defaults from Table B-7 and User-defined. The conditional default and non-default options for KCk, Ymist, and ED are presented in the tables below. Be sure to read the <u>ChemSTEER Estimation Methods and Models</u> topic for more information about changing model parameters.

You may not change the defining model parameter, KCk, to be anything other than the default shown in Table B-7a. If you wish to model inhalation exposures to mists using your own concentration data, choose the <u>User-Defined Inhalation Model</u> or the <u>OSHA PEL-Limiting Model for Substance-Specific</u> <u>Particulates</u>.

**NOTE:** It is assumed that the same number of workers exposed by inhaling the chemical during the activity will also be dermally exposed (if a dermal exposure is expected). If you update the number of workers exposed (NWexp), the NWexp for the corresponding output in the dermal model, selected for the same activity, will be automatically updated with the entered value. For

example, if you update NWexp for Output 2 in this model, NWexp for Output 2 in the dermal model will be updated to the same value. The same is true if you update NWexp for Output 1.

#### Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default characterization for Output 1: *What-If* Default characterization for Output 2: *What-If* 

You may select an alternative characterization for either of the outputs at any time.

#### **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Exposure Model Information* screen:

"EPA/OPPT Automobile OEM Spray Coating Inhalation Model (non-volatile non-polyisocyanates)"

# Table B-7a. KCk for the EPA/OPPT Automobile OEM Spray Coating Inhalation Exposure Model (non-volatile non-polyisocyanates)

Spray Gun Type (from the Shared Parameters/Factors subtab of the Operation Parameters tab)	KCk Default (mg/m³) (Origin Label)	Non-Default Options for KCk <sup>1</sup> (Origin Label)
Conventional <sup>2</sup>	2.3 (Conv/Downdraft)	15 (Conv/Crossdraft) 15 (HVLP/Crossdraft) 1.9 (HVLP/Downdraft)
HVLP	1.9 (HVLP/Downdraft)	15 (HVLP/Crossdraft) 15 (Conv/Crossdraft) 2.3 (Conv/Downdraft)

1. The non-default options for KCk may be selected <u>at the model level</u>. If the value for KCk is changed in the Exposures tab, the new value will only be used in the calculations performed by the model for the selected exposure activity. The spray gun type shared parameter will not be updated in the Shared Parameters/Factors subtab if an alternative KCk value is chosen in the Exposures tab.

2. Conventional spray guns are selected as the default for the Automobile OEM Spray Coating operation in the Shared Parameters/Factors subtab. The conventional spray gun default for the Automobile OEM Spray Coating Operation was adopted as an internal policy decision in July 2003. This setting is also the default for all non-automobile spray coating operations (i.e., the User-Defined operations).

Operation	Ymist Default*	Non-default Options for Ymist**
Automobile OEM Spray Coating	Yfpaint (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Ymist
Automobile Refinish Spray Coating	Yfpaint (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yppaint User-defined Ymist
Not Automobile Spray Coating	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Ymist

Table B-7b. Conditional Default Values for Ymist for the EPA/OPPT Automobile OEM Spray Coating
Inhalation Exposure Model (non-volatile non-polyisocyanates)

\*The default value for Ymist <u>in all cases</u> is the weight fraction of the chemical in the sprayed coating. Yfpaint and Yprod are synonymous to the weight fraction of chemical contained in the product, in its final formulation and as sprayed. Yfpaint is used in the Automobile Spray Coating Operations and Yprod is used by all user-defined operations.

\*\*Non-default options for Ymist are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab. Yrm and Yppaint are synonymous to the weight fraction of the chemical contained in the raw material or coating, as purchased in its initial formulation. Yrm is used in the Automobile OEM Spray Coating Operation, as well as all user-defined operations; Yppaint is used in the Automobile Refinish Spray Coating Operation.

If you enter a User-defined Ymist or Ysf (0 < Ymist < 1, 0 < Ysf < 1) and the value is not valid, ChemSTEER will display a pop-up message warning you that the choice is invalid. You must enter a value that will result in a valid Ymist or Ysf before ChemSTEER will allow you to move on from the selection process.

# Table B-7c. Conditional Default Values for ED for the EPA/OPPT Automobile OEM Spray Coating Inhalation Exposure Model (non-volatile non-polyisocyanates)

Batch Condition	Conditional ED Default (days of exposure/site-yr)	Non-default Options for ED*
Continuous	Lesser of 250 or OD (from Mass Balance subtab of the Operation Parameters tab)	User-defined ED
Batch Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or Nby (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD (days/site-yr) User-defined ED
Batch Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or OD (from the Mass Balance Parameters subtab of the Operation Parameters tab)	Nby (bt/site-yr) User-defined ED

\*Non-default options for ED are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab.

# Key Rationale for Model

Midpoint sampling period TWA values for particulate from several monitoring studies of workers in conditions using the variety of controls noted.

## References

SAIC for US EPA/OPPT/CEB. Generic Scenario for Automobile Spray Coating Draft Report. August 1996.

US EPA/OPPT/CEB. Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991. (Equations 4-1, 4-11)

US EPA Memo entitled Draft Guidance on LADDs and APDRs from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93.

# EPA/OPPT Automobile Refinish Spray Coating Inhalation Exposure Model

#### **Model Description**

This model estimates the amount of non-volatile non-polyisocyanate chemical in mist inhaled by a worker spray painting automobiles in automobile refinish coating operations. This model uses mist concentration data based upon spray gun type and booth type.

## Sources/Activities That Use This Model as a Default

The EPA/OPPT Automobile Refinish Spray Coating Inhalation Exposure Model (non-volatile, non-polyisocyanates) is the default for calculating worker exposures to a non-volatile, non-polyisocyanate chemical during the <u>Automobile Refinish Spray Coating Application</u> source/activity.

This model is not used as an alternative inhalation exposure model for any other sources/activities.

#### Potential Route / Form(s) of Exposure

Inhalation / Particulate or non-volatile portion of mist, aerosols, etc.

#### Equations

Parameters	Description	Equation	Units
Cm	Mass concentration of chemical in air	KCk x Ys	mg/m <sup>3</sup>
1	Inhalation potential dose rate	Cm x b x h	mg/day
NW	Total number of workers exposed	NWexp x NS	workers
LADD	Lifetime average daily dose	(I x ED x EY)/(BW x ATc x 365 days/yr)	mg/kg-day
ADD	Average daily dose	(I x ED x EY)/(BW x AT x 365 days/yr)	mg/kg-day
APDR	Acute potential dose rate	I/BW	mg/kg-day

#### **Model Input Parameters and Default Values**

The EPA/OPPT Automobile Refinish Spray Coating Inhalation Exposure Model default values for each of the input parameters are summarized in Table B-8.

Table B-8. Input Parameters and Default Values for the EPA/OPPT Automobile Refinish Spray Coating
Inhalation Exposure Model (non-volatile non-polyisocyanates)

Parameter	Description	Default Value(s)	Units
KCk	Mass concentration of total particulate in air	Non-default options specified in Table B-8a	mg/ m <sup>3</sup>
Ys	Weight fraction of the chemical in particulate or solids fraction of mist (0 ≤ Ys ≤ 1)	Lesser of (Ymist/Ysf) or 1 or User-defined Ys	dimensionless
Ymist	Weight fraction of chemical in mist (0 ≤ Ymist ≤ 1)	Non-default options specified in Table B-8b	dimensionless
Ysf	Weight fraction of solids in paint (0 ≤ Ysf ≤ 1)	0.25*	dimensionless
b	Volumetric inhalation rate ( $0 < b \le 7.9$ )	1.25	m³/hr
h	Exposure duration ( $0 \le h \le 24$ )	8	hrs/day
NWexp	Number of workers exposed while performing the activity	3	workers/site
NS	Number or sites	NS (from Mass Balance Parameters subtab of the Operation Parameters tab)	site(s)
ED	Days exposed per year (0 ≤ ED (integer) ≤ 365)	Defaults specified in Table B-8c	days/site-yr
EY	Years of occupational exposure ( $0 \le EY$ )	40	years
BW	Body weight (0 ≤ ATc)	70	kg
ATc	Averaging time over a lifetime (chronic) (0 ≤ ATc)	70	years
AT	Averaging time (EY $\leq$ AT $\leq$ ATc)	EY	years

\*The reference generic scenario suggests a default solids fraction of 0.25. It also states that "'high solids paint' for automobiles can have a solids content of up to 45 to 50 volume percent to top coats...; however, solids content varies widely."

You may elect to change any parameter from Table B-8. If you input a user-defined value for Ys, the values of Ymist and Ysf are not used in the model. Clicking the *Type* column for each changeable parameter other than KCk, Ymist, and ED contains only two options: ChemSTEER defaults from Table B-8 and User-defined. The conditional default and non-default options for KCk, Ymist, and ED are presented in the tables below. Be sure to read the <u>ChemSTEER Estimation Methods and Models</u> topic for more information about changing model parameters.

You may not change the defining model parameter, KCk, to be anything other than the defaults shown in Table B-8 and Table B-8a, respectively. If you wish to model inhalation exposures to mists using your own concentration data, choose the <u>User-Defined Inhalation Model</u> or the <u>OSHA PEL-Limiting</u> <u>Model for Substance-Specific Particulates</u>.

**NOTE**: It is assumed that the same number of workers exposed by inhaling the chemical during the activity will also be dermally exposed (if a dermal exposure is expected). If you update the number of workers exposed (NWexp), the NWexp for the corresponding output in the dermal model, selected for the same activity, will be automatically updated with the entered value. For example, if you update NWexp for Output 2 in this model, NWexp for Output 2 in the dermal model will be updated to the same value. The same is true if you update NWexp for Output 1.

## Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default characterization for Output 1: *What-If* Default characterization for Output 2: *What-If* 

You may select an alternative characterization for either of the outputs at any time.

#### **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Exposure Model Information* screen:

"EPA/OPPT Automobile Refinish Spray Coating Inhalation Model (non-volatile non-polyisocyanates)"

# Table B-8a. KCk for the EPA/OPPT Automobile Refinish Spray Coating Inhalation Exposure Model (non-volatile non-polyisocyanates)

Spray Gun Type (from the Shared Parameters/Factors subtab of the Operation Parameters tab)	KCk Default (mg/m <sup>3</sup> ) (Origin Label)	Non-Default Options for KCk <sup>1</sup> (Origin Label)
Conventional <sup>2</sup>	15 (Conv/Downdraft)	15 (HVLP/Crossdraft)
		2.3 (Conv/Downdraft)
		1.9 (HVLP/Downdraft)
HVLP	15 (HVLP/Downdraft)	15 (Conv/Crossdraft)
		2.3 (Conv/Downdraft)
		1.9 (HVLP/Downdraft)

1. The non-default options for KCk may be selected <u>at the model level</u>. If the value for KCk is changed in the Exposures tab, the new value will only be used in the calculations performed by the model for the selected exposure activity. The spray gun type shared parameter will not be updated in the Shared Parameters/Factors subtab if an alternative KCk value is chosen in the Exposures tab.

2. Conventional spray guns are selected as the default for the Automobile Refinish Spray Coating operation in the Shared Parameters/Factors subtab. This setting is also the default for all non-automobile spray coating operations (i.e., the User-Defined operations).

Operation	Ymist Default*	Non-default Options for Ymist**
Automobile Refinish Spray Coating	Yfpaint (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yppaint User-defined Ymist
Automobile OEM Spray Coating	Yfpaint (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Ymist
Not Automobile Spray Coating	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Ymist

# Table B-8b. Conditional Default Values for Ymist for the EPA/OPPT Automobile Refinish Spray Coating Inhalation Exposure Model (non-volatile non-polyisocyanates)

\*The default value for Ymist <u>in all cases</u> is the weight fraction of the chemical in the sprayed coating. Yfpaint and Yprod are synonymous to the weight fraction of chemical contained in the product, in its final formulation and as sprayed. Yfpaint is used in the Automobile Spray Coating Operations and Yprod is used by all user-defined operations.

\*\*Non-default options for Ymist are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab. Yrm and Yppaint are synonymous to the weight fraction of the chemical contained in the raw material or coating, as purchased in its initial formulation. Yrm is used in the Automobile OEM Spray Coating Operation, as well as all user-defined operations; Yppaint is used in the Automobile Refinish Spray Coating Operation.

If you enter a User-defined Ymist or Ysf (0 < Ymist < 1, 0 < Ysf < 1) and the value is not valid, ChemSTEER will display a pop-up message warning you that the choice is invalid. You must enter a value that will result in a valid Ymist or Ysf before ChemSTEER will allow you to move on from the selection process.

# Table B-8c. Conditional Default Values for ED for the EPA/OPPT Automobile Refinish Spray Coating Inhalation Exposure Model (non-volatile non-polyisocyanates)

Batch Condition	Conditional ED Default (days of exposure/site-yr)	Non-default Options for ED*
Continuous	Lesser of 250 or OD (from Mass Balance subtab of the Operation Parameters tab)	User-defined ED
Batch Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or Nby (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD (days/site-yr) User-defined ED
Batch Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or OD (from the Mass Balance Parameters subtab of the Operation Parameters tab)	Nby (bt/site-yr) User-defined ED

\*Non-default options for ED are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab.

# Key Rationale for Model

Midpoint sampling period TWA values for particulate from several monitoring studies of workers in conditions using the variety of controls noted.

## References

SAIC for US EPA/OPPT/CEB. Generic Scenario for Automobile Spray Coating Draft Report. August 1996.

Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991. (Equations 4-1, 4\_11)

US EPA Memo entitled Draft Guidance on LADDs and APDRs from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93.

# EPA/OPPT Automobile Spray Coating Inhalation Exposure Model

#### **Model Description**

This model estimates the amount of polyisocyanate chemical in mist inhaled by a worker spray painting automobiles or similar applications. This model uses mist concentration data based upon conventional spray guns used in crossdraft booths by default.

## Sources/Activities That Use This Model as a Default

There are no sources/activities in ChemSTEER that use this model as a default for calculating worker inhalation exposures to a chemical.

# **Other Sources/Activities**

The EPA/OPPT Automobile Spray Coating Inhalation Exposure Model (non-volatile polyisocyanates) Model may be an appropriate means to calculate worker inhalation exposures to a non-volatile polyisocyante chemical while performing either of the <u>Automobile Spray Coating</u> sources/activities.

#### Potential Route / Form(s) of Exposure

Inhalation / Particulate or non-volatile portion of mist, aerosols, etc.

Parameters	Description	Equation	Units
Cm	Mass concentration of chemical in air	KCk	mg/m <sup>3</sup>
1	Inhalation potential dose rate	Cm x b x h	mg/day
NW	Total number of workers exposed	NWexp x NS	workers
LADD	Lifetime average daily dose	(I x ED x EY)/(BW x ATc x 365 days/yr)	mg/kg-day
ADD	Average daily dose	(I x ED x EY)/(BW x AT x 365 days/yr)	mg/kg-day
APDR	Acute potential dose rate	I/BW	mg/kg-day

## Equations

## **Model Input Parameters and Default Values**

The EPA/OPPT Automobile Spray Coating Inhalation Exposure Model (polyisocyanates) default values for each of the input parameters are summarized in Table B-9.

Parameter	Description	Default Value(s)	Units
KCk	Mass concentration of total particulate in air	Non-default options specified in Table B-9a	mg/ m <sup>3</sup>
b	Volumetric inhalation rate (0 < b ≤ 7.9)	1.25	m³/hr
h	Exposure duration ( $0 \le h \le 24$ )	8	hrs/day
NWexp	Number of workers exposed while performing the activity	3	workers/site
NS	Number or sites	NS (from Mass Balance Parameters subtab of the Operation Parameters tab)	site(s)
ED	Days exposed per year (0 ≤ ED (integer) ≤ 365)	Defaults specified in Table B-4c	days/site-yr
EY	Years of occupational exposure (0 ≤ EY)	40	years
BW	Body weight (0 ≤ ATc)	70	kg
ATc	Averaging time over a lifetime (chronic) (0 ≤ ATc)	70	years
AT	Averaging time (EY $\leq$ AT $\leq$ ATc)	EY	years

Table B-9. Input Parameters and Default Values for the EPA/OPPT Automobile Spray Coating
Inhalation Exposure Model (polyisocyanates)

You may elect to change any parameter from Table B-9. Clicking the *Type* column for each changeable parameter other than KCk and ED contains only two options: ChemSTEER defaults from Table B-9 and User-defined. The conditional default and non-default options for KCk and ED are presented in the tables below. Be sure to read the <u>ChemSTEER Estimation Methods and Models</u> topic for more information about changing model parameters.

You may not change the defining model parameter, KCk, to be anything other than the default shown in Table B-9a. If you wish to model inhalation exposures to mists using your own concentration data, choose the <u>User-Defined Inhalation Model</u> or the <u>OSHA PEL-Limiting Model for Substance-Specific</u> <u>Particulates</u>.

**NOTE**: It is assumed that the same number of workers exposed by inhaling the chemical during the activity will also be dermally exposed (if a dermal exposure is expected). If you update the number of workers exposed (NWexp), the NWexp for the corresponding output in the dermal model, selected for the same activity, will be automatically updated with the entered value. For example, if you update NWexp for Output 2 in this model, NWexp for Output 2 in the dermal model will be updated to the same value. The same is true if you update NWexp for Output 1.

#### Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: Enabled

Enable Model Parameters for Output 2: Enabled

Default characterization for Output 1: *What-If* Default characterization for Output 2: *What-If* 

You may select an alternative characterization for either of the outputs at any time.

## **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Exposure Model Information* screen:

"EPA/OPPT Automobile Spray Coating Inhalation Model (non-volatile polyisocyanates)"

# Table B-9a. KCk Options for the EPA/OPPT Automobile Spray Coating Inhalation Exposure Model (polyisocyanates)

Spray Gun Type (from the Shared Parameters/Factors subtab of the Operation Parameters tab)	KCk Default (mg/m³) (Origin Label)		Non-Default Oı (Origin	otions for K Label)	'Ck <sup>1</sup>	
	Origin Label	Output 1	Output 2	Selection/Origin Label	Output 1	Output 2
Conventional <sup>2</sup>	Conv/Crossdraft	0.05	18.4	HVLP/Crossdraft Conv/ Downdraft HVLP/Downdraft	1.0 0.01 0.6	5.2 3.7 1.4
HVLP	HVLP/Crossdraft	1.0	5.2	Conv/Crossdraft Conv/Downdraft HVLP/Downdraft	0.05 0.01 0.6	18.4 3.7 1.4

1. The non-default options for KCk may be selected <u>at the model level</u>. If the value for KCk is changed in the Exposures tab, the new value will only be used in the calculations performed by the model for the selected exposure activity. The spray gun type shared parameter will not be updated in the Shared Parameters/Factors subtab if an alternative KCk value is chosen in the Exposures tab.

2. The Shared Parameters/Factors subtab defaults to the conventional spray gun for all operations (Auto Spray Coating and User-defined).

Table B-9b. Conditional Default Values for ED for the EPA/OPPT Automobile Spray Coating Inhalation			
Exposure Model (polyisocyanates)			

Batch Condition	Conditional ED Default (days of exposure/site-yr)	Non-default Options for ED*
Continuous	Lesser of 250 or OD (from Mass Balance subtab of the Operation Parameters tab)	User-defined ED
Batch Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or Nby (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD (days/site-yr) User-defined ED
Batch Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or OD (from the Mass Balance Parameters subtab of the Operation Parameters tab)	Nby (bt/site-yr) User-defined ED

\*Non-default options for ED are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab.

#### **Key Rationale for Model**

Measured or estimated concentration ranges for particulate from several monitoring studies of workers in conditions using the variety of controls noted.

#### References

SAIC for US EPA/OPPT/CEB. Generic Scenario for Automobile Spray Coating Draft Report. August 1996.

Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991. (Equations 4-1, 4-11)

US EPA Memo entitled Draft Guidance on LADDs and APDRs from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93.

# EPA/OPPT UV Roll Coating Inhalation Model

#### **Model Description**

This model estimates the amount of chemical inhaled by a worker who conducts activities near roll coater(s) using coatings or inks containing the chemical.

#### Sources/Activities That Use This Model as a Default

The EPA/OPPT UV Roll Coating Inhalation Model is the default for calculating worker inhalation exposures to a chemical while performing the <u>Roll Coating</u> source/activity.

**Other Sources/Activities** 

The EPA/OPPT UV Roll Coating Inhalation Model may be an appropriate alternative to the default inhalation model for the following sources/activities:

- Miscellaneous Sources/Activities Related to Liquid Processing
- <u>Miscellaneous Sources/Activities Related to Solid Processing</u>

## Potential Route / Form(s) of Exposure

Inhalation / Particulate or non-volatile portion of mist, aerosols, etc.

#### Equations

Parameters	Description	Equation	Units
Cm	Mass concentration of chemical in air	KCk x Ys	mg/m <sup>3</sup>
1	Inhalation potential dose rate	Cm x b x h	mg/day
NW	Total number of workers exposed	NWexp x NS	workers
LADD	Lifetime average daily dose	(I x ED x EY)/(BW x ATc x 365 days/yr)	mg/kg-day
ADD	Average daily dose	(I x ED x EY)/(BW x AT x 365 days/yr)	mg/kg-day
APDR	Acute potential dose rate	I/BW	mg/kg-day

## **Model Input Parameters and Default Values**

The EPA/OPPT UV Roll Coating Inhalation Model default values for each of the input parameters are summarized in Table B-10.

Parameter	Description	Default Value(s)	Units
KCk	Mass concentration of total particulate or nonvolatile portion of mist in air (based on data)	Output 1: <u>Default:</u> 0.04 (Low end of range) <u>Non-default Option:</u> 0.26 (High end of range)	mg/ m <sup>3</sup>
		Output 2: <u>Default:</u> 0.26 (High end of range) <u>Non-default Option:</u> 0.04 (Low end of range)	
Ys	Weight fraction of chemical in particulate or non-volatiles fraction of mist $(0 \le Ys \le 1)$	Lesser of (Ymist/Ysf) or 1	dimensionless
Ymist	Weight fraction of chemical in mist (0 ≤ Ymist ≤ 1)	Non-default options specified in Table B-10a	dimensionless
Ysf	Weight fraction of solids in coating ( $0 \le Ysf \le 1$ )	0.25*	dimensionless
b	Volumetric inhalation rate ( $0 < b \le 7.9$ )	1.25	m³/hr
h	Exposure duration ( $0 \le h \le 24$ )	8	hrs/day
NWexp	Number of workers exposed while performing the activity	1	workers/site
NS	Number or sites	NS (from Mass Balance Parameters subtab of the Operation Parameters tab)	site(s)
ED	Days exposed per year (0 ≤ ED (integer) ≤ 365)	Defaults specified in Table B-10b	days/site-yr
EY	Years of occupational exposure ( $0 \le EY$ )	40	years
BW	Body weight (0 ≤ ATc)	70	kg
ATc	Averaging time over a lifetime (chronic) (0 ≤ ATc)	70	years
AT	Averaging time (EY $\leq$ AT $\leq$ ATc)	EY	years

Table B-10. In	out Parameters an	d Default Values	for the EPA/C	OPPT UV Roll Co	pating Inhalation Model
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\*The default solids (i.e., non-volatiles) fraction in this model is based on information contained in the *1996 Generic Scenario for Automobile Spray Coating*. This reference also states that "'high solids paint' for automobiles can have a solids content of up to 45 to 50 volume percent to top coats...; however, solids content varies widely." Specific data for UV/EB-curable roll coatings is not currently available. If you have data to suggest an alternative value, you are encouraged to use it in the calculations.

You may elect to change any parameter from Table B-10 except KCk, which is a constant. Clicking the *Type* column for each changeable parameter other than KCk, Ymist, and ED contains only two options: ChemSTEER defaults from Table B-10 and User-defined. The conditional default and non-default options for Ymist and ED are presented in the tables below. Be sure to read the <u>ChemSTEER</u> <u>Estimation Methods and Models</u> topic for more information about changing model parameters.

You may not change the defining model parameter, KCk, to be anything other than the default shown in Table B-10a. If you wish to model inhalation exposures to solids or mists using your own data or based on OSHA PELs, choose one of the following alternative models:
OSHA PEL-Limiting Model for Substance-Specific Particulates; OSHA Total PNOR PEL-Limiting Model; or User-Defined Inhalation Model.

**NOTE**: It is assumed that the same number of workers exposed by inhaling the chemical during the activity will also be dermally exposed (if a dermal exposure is expected). If you update the number of workers exposed (NWexp), the NWexp for the corresponding output in the dermal model, selected for the same activity, will be automatically updated with the entered value. For example, if you update NWexp for Output 2 in this model, NWexp for Output 2 in the dermal model will be updated to the same value. The same is true if you update NWexp for Output 1.

## Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Enabled* Enable Model Parameters for Output 2: *Enabled* 

Default Characterization of Output 1 Results: *Low end of range* Default Characterization of Output 2 Results: *High end of range* 

You may select an alternative characterization for either of the outputs at any time.

## **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Exposure Model Information* screen:

"EPA/OPPT UV Roll Coating Inhalation Model (non-volatiles); airborne particulate concentration (KCk) is based on 8-hour TWA personal monitoring data"

**NOTE:** If you click in the Basis text box and modify the default text, the dynamic text will no longer function. You will be required to manually update the text box.

Operation	Ymist Default*	Non-default Options for Ymist**
Automobile OEM Spray Coating	Yfpaint (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Ymist
Automobile Refinish Spray Coating	Yfpaint (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yppaint User-defined Ymist
Not Automobile Spray Coating	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Ymist

## Table B-10a. Conditional Default Values for Ymist for the EPA/OPPT UV Roll Coating Inhalation Model

\*The default value for Ymist <u>in all cases</u> is the weight fraction of the chemical in the rolled coating or ink. Yfpaint and Yprod are synonymous to the weight fraction of chemical contained in the product, in its final formulation and as applied. Yfpaint is used in the Automobile Spray Coating Operations and Yprod is used by all user-defined operations.

\*\*Non-default options for Ymist are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab. Yrm and Yppaint are synonymous to the weight fraction of the chemical contained in the raw material or coating, as purchased in its initial formulation. Yrm is used in the Automobile OEM Spray Coating Operation, as well as all user-defined operations; Yppaint is used in the Automobile Refinish Spray Coating Operation.

If you enter a User-defined Ymist or Ysf (0 # Ymist # 1, 0 # Ysf # 1) and the value is not valid, ChemSTEER will display a pop-up message warning you that the choice is invalid. You must enter a value that will result in a valid Ymist or Ysf before ChemSTEER will allow you to move on from the selection process.

Batch Condition	Conditional ED Default (days of exposure/site-yr)	Non-default Options for ED*
Continuous	Lesser of 250 or OD (from Mass Balance subtab of the Operation Parameters tab)	User-defined ED
Batch Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or Nby (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD (days/site-yr) User-defined ED
Batch Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or OD (from the Mass Balance Parameters subtab of the Operation Parameters tab)	Nby (bt/site-yr) User-defined ED

#### Table B-10b. Conditional Default Values for ED for the EPA/OPPT UV Roll Coating Inhalation Model

\*Non-default options for ED are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab.

## **Key Rationale for Model**

Limited personal samples from a monitoring study of workers in exposed to 'ink fly' in a facility using offset lithographic printing of cartonboard using UV-curable ink, which may be applied to similar

roll coating operations. This model assumes that the exposure concentration is the same as the concentration of the chemical in the non-volatile portion of the coating mixture.

## References

Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991. (Equations 4-1, 4-11)

US EPA Memo entitled Draft Guidance on LADDs and APDRs from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93.

SAIC for US EPA/OPPT/CEB. Generic Scenario for Automobile Spray Coating Draft Report. August 1996.

Generic Scenario: Roll Coating of UV-Curable Coatings. No date.

## User-Defined Inhalation Model

#### **Model Description**

This model estimates the amount of chemical inhaled by a worker during an activity. Estimation of the concentration for inhalation exposure is based on a user input concentration.

#### Sources/Activities That Use This Model as a Default

The following sources/activities use the User-Defined Inhalation Model as the default for calculating worker inhalation exposures:

- Miscellaneous Sources/Activities Related to Liquid Processing
- Aqueous Wash of Organic Mass
- <u>Scrubber Releases</u>
- Coating Using Hand Held Spray Can

This model is appropriate to use as an alternative inhalation model for <u>all</u> other ChemSTEER sources/activities (except the *Recirculating Water-Cooling Tower Additive Releases* source/activity).

## Potential Route / Form(s) of Exposure

Inhalation / Vapor, particulate, mist, aerosols, etc.

NOTE: The model will default to Chemical State = 'Mist' when the adjusted vapor pressure of the substance being handled (e.g., AVPrm, AVPprod) (calculated on the *Operation Parameters* tab, *Shared Parameters/Factors* subtab) is outside of the preferred range of adjusted vapor pressures (i.e., is less than AVPlow). To read more about these settings, refer to the following topics:

Vapor Model Activation

Operation Parameters Tab → Shared Parameters/Factors Subtab

Parameters	Description	Equation	Units
Cm	Mass concentration of chemical in air	Cv x MW / Vm x Ys	mg/m <sup>3</sup>
1	Inhalation potential dose rate	Cm x b x h	mg/day
NW	Total number of workers exposed	NWexp x NS	workers
LADD	Lifetime average daily dose	(I x ED x EY)/(BW x ATc x 365 days/yr)	mg/kg-day
ADD	Average daily dose	(I x ED x EY)/(BW x AT x 365 days/yr)	mg/kg-day
APDR	Acute potential dose rate	I/BW	mg/kg-day

## Equations

#### **Model Input Parameters and Default Values**

The User-Defined Inhalation Model default values for each of the input parameters are summarized in Table B-11.

Parameter	Description	Default Value(s)	Units
Cv	Volumetric concentration of chemical in air ( $0 \le Cv$ )	User-defined Cv	ppm
MW	Molecular weight of the chemical (0 $\leq$ MW)	MW (from Chemical tab)	g/mol
Vm	Molar volume (0 ≤ Vm)	24.45 @ 25°C, 1 atm	L/mol
Cm	Mass concentration of chemical in air $(0 \le Cm)$	Calculated from model equation or User- defined Cm	mg/m <sup>3</sup>
Ys	Weight fraction of chemical in mixture $(0 \le Yx \le 1)^1$	1	dimensionless
b	Volumetric inhalation rate (0 < b ≤ 7.9)	1.25	m <sup>3</sup> /hr
h	Exposure duration ( $0 \le h \le 24$ )	Defaults specified in Table B-11a	hrs/day
NWexp	Number of workers exposed while performing the activity	1	workers/site
NS	Number or sites	NS (from Mass Balance Parameters subtab of the Operation Parameters tab)	site(s)
ED	Days exposed per year (0 ≤ ED (integer) ≤ 365)	Defaults specified in Table B-11b	days/site-yr
EY	Years of occupational exposure (0 ≤ EY)	40	years
BW	Body weight (0 ≤ ATc)	70	kg
ATc	Averaging time over a lifetime (chronic) (0 ≤ ATc)	70	years
AT	Averaging time (EY $\leq$ AT $\leq$ ATc)	EY	years

Table B-11. Input Parameters and Default Values for the User-Defined Inhalation Mode
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1. Ys may be used to adjust the airborne concentration, as appropriate.

You may elect to change any parameter from Table B-11. If you enter a user-defined value for Cm, the values of Cv, MW, and Vm are not used in the model. Clicking the *Type* column for each

changeable parameter other than Cv, Cm, Ys, h, and ED contains only two options: ChemSTEER defaults from Table B-11 and User-defined. You <u>must</u> enter a value for Cv or Cm in this exposure model. The conditional default and non-default options for h and ED are presented in the tables below. Be sure to read the <u>ChemSTEER Estimation Methods and Models</u> topic for more information about changing model parameters.

The non-default options for Ys are Yrm, Yprod, Yi (for container-related sources/activities only), and User-defined Ys. These non-default options are available by clicking in the *Type* column in the *View/Update Exposure Model Information* screen in the Exposures tab.

**NOTE**: It is assumed that the same number of workers exposed by inhaling the chemical during the activity will also be dermally exposed (if a dermal exposure is expected). If you update the number of workers exposed (NWexp), the NWexp for the corresponding output in the dermal model, selected for the same activity, will be automatically updated with the entered value. For example, if you update NWexp for Output 2 in this model, NWexp for Output 2 in the dermal model will be updated to the same value. The same is true if you update NWexp for Output 1.

## Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default Characterization of Output 1 Results: *Output 1* Default Characterization of Output 2 Results: *Output 2* 

You may select an alternative characterization for either of the outputs at any time.

## Default Model Basis

The following default text is displayed in the *Basis* box on the *View/Update Exposure Model Information* screen:

"User-Defined Inhalation Model"

Associated Release Model	Source / Activity Type	Conditional h Default* (hrs/site-day)
Yes	Any type	Lesser of 8 or OHa from an associated release model** (from Releases tab)
No	Container-Related	Lesser of 8 or OHa (from Container Parameters subtab of the Operation Parameters tab)
	Sampling	1
	Equipment Cleaning Losses of Liquids from Multiple Vessels	4
	Equipment Cleaning Losses of Liquids from a Single, Large Vessel	1
	Equipment Cleaning Losses of Liquids from a Single, Small Vessel	0.5
	Not Container-Related, Sampling, or Equipment Cleaning	8

Table B-11a. Conditional Default Values for h for the User-Defined Inhalation Model

\*See Table B-11c for the hierarchy of logic for extracting an h value from an associated release model.

Associated Release Model / Source/Activity Type / Operation Mode	Batch Condition	Conditional ED Default (days of exposure/site-yr)	Non-default Options for ED**
Yes / Container-related / Continuous	Not applicable	Lesser of 250 or Freq from associated release model* (from Releases tab)	OD (days/site- yr) ODa (days/site- yr) User-defined ED
Yes / Container-related / Batch	Any	Lesser of 250 or Freq from associated release model* (from Releases tab)	Nby (bt/site-yr) OD (days/site- yr) ODa (days/site- yr) User-defined ED
Yes / Not Container-related / Continuous	Not applicable	Lesser of 250 or Freq from associated release model* (from Release tab)	OD (days/site- yr) User-defined ED
Yes / Not Container-related / Batch	Any	Lesser of 250 or Freq from associated release model* (from Releases tab)	Nby (bt/site-yr) OD (days/site- yr) User-defined ED
No associated release model / Container-Related / Continuous	Not applicable	Lesser of 250 or ODa (from Container Parameters subtab of the Operations Parameters tab)	OD (das/site-yr) User-defined ED
No associated release model /Container-Related /Batch	Any	Lesser of 250 or ODa (from Container Parameters subtab of the Operations Parameters tab)	Nby (bt/site-yr) OD (days/st-yr) User-defined ED
No associated release model / Not Container-Related /Continuous	Not applicable	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	User-defined ED
No associated release model / Not Container-Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or Nby (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD (days/site- yr) User-defined ED
	Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby (bt/site-yr) User-defined ED

Table B-11b. Conditional Default Values for ED for the User-Defined Inhalation Model

\*See Table B-11c for the hierarchy of logic for extracting an ED value from an associated release model.

\*\*Non-default options for ED are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab.

## Table B-11c. Hierarchy for Extracting Parameter Defaults from Associated Release Models\* for the User-Defined Inhalation Model

- 1. Use current value of parameter from the last associated vapor generation model\* for the source/activity (from the Releases tab).
- 2. Use current value of parameter from the last associated release model\* for the source/activity (from the Releases tab) only if there is not associated vapor generation model.
- 3. If no associated release model\* for the source/activity, then use conditional default as described for "No associated release model" in Tables B-11a and B-11b above.

\*The associated release model is the LAST vapor generation or release model that contains a parameter value required for the EPA/OPPT Mass Balance Inhalation Model that is listed in the *Release Model(s)* for Selected Activity box in the Releases tab (i.e., it is the last vapor generation or release model that was added by either ChemSTEER or the user) for the selected Source/Activity.

When extracting parameter values from the Releases tab, the *EPA/OPPT User-Defined Inhalation Model* Input Parameters for Output 1 are obtained from the associated release model Input Parameters for Output 1; and the *EPA/OPPT User-Defined Inhalation Model* Input Parameters for Output 2 are obtained from the associated release model Input Parameters for Output 2.

## Key Rationale for Model

NA

## References

US EPA/OPPT/CEB. Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991. (Equations 4-1, 4-5)

US EPA Memo entitled Draft Guidance on LADDs and APDRs from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93.

Models for Calculating Dermal Exposures

## EPA/OPPT 1-Hand Dermal Contact with Liquid Model

## **Model Description**

This model estimates dermal exposure to the chemical for 1-hand contact with liquid containing the chemical.

## Sources/Activities That Use This Model as a Default

The EPA/OPPT 1-Hand Dermal Contact with Liquid Model is the default for calculating worker dermal exposures to a liquid chemical while performing <u>Sampling Liquids</u> sources/activities.

## EPA/OPPT 1-Hand Dermal Contact with Liquid Model – Other Sources/Activities

The EPA/OPPT 1-Hand Dermal Contact with Liquid Model may be an appropriate alternative to the default dermal model for the following sources/activities:

- All sources/activities for <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>
- All sources/activities for Loading Liquids into Transport Containers/Vessels
- All sources/activities for <u>Unloading Liquids from Transport Containers/Vessels</u>
- All sources/activities for Equipment Cleaning Losses of Liquids
- <u>Miscellaneous Sources/Activities Related to Liquid Processing</u>
- Filter Media Changeout

## Potential Route / Form(s) of Exposure

Dermal contact / Liquid

#### Equations

Parameters	Description	Equation	Units
Dexp	Dermal potential dose rate	S x Qu x Yderm x FT	mg/day
NW	Total number of workers exposed	NWexp x NS	workers
LADD	Lifetime average daily dose	(Dexp x ED x EY)/(BW x ATc x 365 days/yr)	mg/kg-day
ADD	Average daily dose	(Dexp x ED x EY)/(BW x AT x 365 days/yr)	mg/kg-day
APDR	Acute potential dose rate	Dexp/BW	mg/kg-day

## **Model Input Parameters and Default Values**

The EPA/OPPT 1-Hand Dermal Contact with Liquids Model default values for each of the input parameters are summarized in Table B-12.

Parameter	Description	Default Value(s)	Units
S	Surface area of contact (one hand) (constant)	535 (mean)	cm <sup>2</sup>
Qu	Quantity remaining on skin (constant)	Output 1: <u>Default:</u> 0.7 (low) <u>Non-default option:</u> 2.1 (high) Output 2: <u>Default:</u> 2.1 (high) <u>Non-default Option:</u> 0.7 (low)	mg/cm <sup>2</sup> -event
Yderm	Weight fraction of chemical in liquid (0 ≤ Yderm ≤ 1)	Defaults specified in Table B-12a	dimensionless
FT	Frequency of events (0 ≤ FT (integer)	1	events/worker-day
NWexp	Number of workers exposed while performing the activity	1	workers/site
NS	Number or sites	NS (from Mass Balance Parameters subtab of the Operation Parameters tab)	site(s)
ED	Days exposed per year (0 ≤ ED (integer) ≤ 365)	Defaults specified in Table B-12b	days/site-yr
EY	Years of occupational exposure (0 ≤ EY)	40	years
BW	Body weight (0 ≤ ATc)	70	kg
ATc	Averaging time over a lifetime (chronic) (0 ≤ ATc)	70	years
AT	Averaging time (EY ≤ AT ≤ ATc)	EY	years

## Table B-12. Input Parameters and Default Values for the EPA/OPPT 1-Hand Dermal Contact with Liquids Model

You may elect to change any parameter from Table B-12 except S and Qu, which are constants. Clicking the *Type* column for each changeable parameter other than S, Qu, Yderm and ED contains only two options: ChemSTEER defaults from Table B-12 and User-defined. The conditional default and nondefault options for Yderm and ED are presented in the tables below. Be sure to read the <u>ChemSTEER</u> <u>Estimation Methods and Models</u> topic for more information about changing model parameters.

Note on FT: Only one contact per day (FT = 1) is assumed because Qu, with few exceptions, is not expected to be significantly affected either by wiping excess from skin or by repeated contact(s) with additional chemical (i.e., wiping excess from the skin does not remove a significant fraction of the small layer of chemical adhering to the skin and additional contacts with the chemical do not add a significant fraction to the layer). Exceptions to this assumption may be considered for chemicals with high volatility and/ or with very high rates of absorption into the skin.

If you enter a User-defined FT and the value is greater than 1, ChemSTEER will display a warning message with the following text: "The value of FT should not exceed 1 unless the chemical assessed is

highly volatile or has a high rate of absorption. See the *Note on FT* in the User Guide topic for any dermal model for more information on this issue." After clicking "OK" you will be allowed to continue.

You may not change the defining model parameters, Qu and S, to be anything other than the defaults shown above. If you wish to model dermal exposures using your own data, choose the <u>US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.</u> User-Defined Dermal Model.

**NOTE**: It is assumed that the same number of workers dermally exposed to the chemical during the activity will also have an inhalation exposure (if an inhalation exposure is expected). If you update the number of workers exposed (NWexp), the NWexp for the corresponding output in the inhalation model, selected for the same activity, will be automatically updated with the entered value. For example, if you update NWexp for Output 2 in this model, NWexp for Output 2 in the inhalation model will be updated to the same value. The same is true if you update NWexp for Output 1.

## Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Settings for either Output 1 or Output 2 results are based on which Qu is selected for the corresponding output:

- Results using the low remaining quantity (Qu) are characterized as *Output 1* by default.
- Results using the high remaining quantity (Qu) are characterized as *High End* by default.

You may select an alternative characterization for either of the outputs at any time.

## **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Exposure Model Information* screen:

"EPA/OPPT 1-Hand Dermal Contact with Liquids Model"

Source/Activity Type / Material Named in Source/Activity Label	Operation Type	Conditional Yderm Default	Non-default Options for Yderm
Container-Related / Any	Any	Yi (from the Container Parameters subtab of the Operation Parameters tab)	Yrm Yprod User-defined Yderm
Not Container-Related / Raw Material	Any	Yrm (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Yderm
Not Container Related / Product	Any	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Yderm
Not Container-Related / Neither Raw Material nor Product	Manufacturing	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Yderm
	Processing Use	Yrm (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Yderm

# Table B-12a. Conditional Default Values for Yderm for the EPA/OPPT 1-Hand Dermal Contact with Liquids Model

\*Non-default options for Yderm are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab. All default and non-default options for Yderm are available for both Output 1 and Output 2.

Source/Activity Type / Operation Mode	Batch Condition	Conditional ED Default (days of exposure/site-yr)	Non-default Options for ED
Container-Related / Continuous	Not applicable	Lesser of 250 or ODa (from Container Parameters subtab of the Operation Parameters tab)	OD (days/site-yr) User-defined ED
Container-Related / Batch	Any	Lesser of 250 or ODa (from Container Parameters subtab of the Operation Parameters tab)	Nby (bt/site-yr) OD (days/site-yr) User-defined ED
Not Container Related / Continuous	Not applicable	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	User-defined ED
Not Container-Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or Nby (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD User-defined ED
	Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby User-defined ED

## Table B-12b. Conditional Default Values for ED for the EPA/OPPT 1-Hand Dermal Contact with Liquids Model

\*Non-default options for ED are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab. All default and non-default options for ED are available for both Output 1 and Output 2.

## Key Rationale for Model

Dermal exposures to a chemical are estimated using standard assumptions documented in the references, and assume no use of controls or gloves to reduce exposures. For a given worker activity, this method assumes a specific surface area contacted by chemical and a specific surface density of that chemical to estimate a PDR using the model equations.

## References

US EPA/OPPT/CEB. Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991. (Equations 4-26)

US EPA Memo entitled Draft Guidance on LADDs and APDRs from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93.

US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.

## EPA/OPPT 2-Hand Dermal Contact with Liquid Model

## **Model Description**

This model estimates dermal exposure to the chemical for 2-hand contact with liquid containing the chemical.

## Sources/Activities That Use This Model as a Default

The EPA/OPPT 2-Hand Dermal Contact with Liquid Model is the default for calculating worker dermal exposures to a liquid chemical while performing the following sources/activities:

- All sources/activities for <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>
- All sources/activities for Loading Liquids into Transport Containers/Vessels
- All sources/activities for <u>Unloading Liquids from Transport Containers/Vessels</u>
- <u>Aqueous Wash of Organic Mass</u>
- Liquid/Liquid Extraction Solvent Disposal

## EPA/OPPT 2-Hand Dermal Contact with Liquid Model – Other Sources/Activities

The EPA/OPPT 2-Hand Dermal Contact with Liquid Model may be an appropriate alternative to the default dermal model for the following sources/activities:

- All sources/activities for Equipment Cleaning Losses of Liquids
- All sources/activities for Sampling Liquids
- Miscellaneous Sources/Activities Related to Liquid Processing
- Filter Media Changeout
- Roll Coating

## Potential Route / Form(s) of Exposure

Dermal contact / Liquid

#### Equations

Parameters	Description	Equation	Units
Dexp	Dermal potential dose rate	S x Qu x Yderm x FT	mg/day
NW	Total number of workers exposed	NWexp x NS	workers
LADD	Lifetime average daily dose	(Dexp x ED x EY)/(BW x ATc x 365 days/yr)	mg/kg-day
ADD	Average daily dose	(Dexp x ED x EY)/(BW x AT x 365 days/yr)	mg/kg-day
APDR	Acute potential dose rate	Dexp/BW	mg/kg-day

## **Model Input Parameters and Default Values**

The EPA/OPPT 2-Hand Dermal Contact with Liquids Model default values for each of the input parameters are summarized in Table B-13.

Parameter	Description	Default Value(s)	Units
S	Surface area of contact (two hands) (constant)	1,070 (mean)	cm <sup>2</sup>
Qu	Quantity remaining on skin (constant)	Output 1: <u>Default:</u> 0.7 (low) <u>Non-default option:</u> 2.1 (high)	mg/cm <sup>2</sup> -event
		Output 2: <u>Default:</u> 2.1 (high) <u>Non-default Option:</u> 0.7 (low)	
Yderm	Weight fraction of chemical in liquid (0 ≤ Yderm ≤ 1)	Defaults specified in Table B-9a	dimensionless
FT	Frequency of events (0 ≤ FT (integer)	1	events/worker-day
NWexp	Number of workers exposed while performing the activity	1	workers/site
NS	Number or sites	NS (from Mass Balance Parameters subtab of the Operation Parameters tab)	site(s)
ED	Days exposed per year (0 ≤ ED (integer) ≤ 365)	Defaults specified in Table B-9b	days/site-yr
EY	Years of occupational exposure (0 ≤ EY)	40	years
BW	Body weight (0 ≤ ATc)	70	kg
ATc	Averaging time over a lifetime (chronic) (0 ≤ ATc)	70	years
AT	Averaging time (EY $\leq$ AT $\leq$ ATc)	EY	years

 Table B-13. Input Parameters and Default Values for the EPA/OPPT 2-Hand Dermal Contact with

 Liquids Model

You may elect to change any parameter from Table B-13 except S and Qu, which are constants. Clicking the *Type* column for each changeable parameter other than S, Qu, Yderm and ED contains only two options: ChemSTEER defaults from Table B-13 and User-defined. The conditional default and non-default options for Yderm and ED are presented in the tables below. Be sure to read the <u>ChemSTEER</u> <u>Estimation Methods and Models</u> topic for more information about changing model parameters.

NOTE on FT: Only one contact per day (FT = 1) is assumed because Qu, with few exceptions, is not expected to be significantly affected either by wiping excess from skin or by repeated contact(s) with additional chemical (i.e., wiping excess from the skin does not remove a significant fraction of the small layer of chemical adhering to the skin and additional contacts with the chemical do not add a significant fraction to the layer). Exceptions to this assumption may be considered for chemicals with high volatility and/ or with very high rates of absorption into the skin.

If you enter a User-defined FT and the value is greater than 1, ChemSTEER will display a warning message with the following text: "The value of FT should not exceed 1 unless the chemical assessed is highly volatile or has a high rate of absorption. See the Note on FT in the User Guide topic for any dermal model for more information on this issue." After clicking "OK" you will be allowed to continue.

You may not change the defining model parameters, Qu and S, to be anything other than the defaults shown above. If you wish to model dermal exposures using your own data, choose the <u>US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.</u> User-Defined Dermal Model.

NOTE: It is assumed that the same number of workers dermally exposed to the chemical during the activity will also have an inhalation exposure (if an inhalation exposure is expected). If you update the number of workers exposed (NWexp), the NWexp for the corresponding output in the inhalation model, selected for the same activity, will be automatically updated with the entered value. For example, if you update NWexp for Output 2 in this model, NWexp for Output 2 in the inhalation model will be updated to the same value. The same is true if you update NWexp for Output 1.

## Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Settings for either Output 1 or Output 2 results are based on which Qu is selected for the corresponding output:

- Results using the low remaining quantity (Qu) are characterized as *Output 1* by default.
- Results using the high remaining quantity (Qu) are characterized as *High End* by default.

You may select an alternative characterization for either of the outputs at any time.

## **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Exposure Model Information* screen:

"EPA/OPPT 2-Hand Dermal Contact with Liquids Model"

Source/Activity Type / Material Named in Source/Activity Label	Operation Type	Conditional Yderm Default	Non-default Options for Yderm
Container-Related / Any	Any	Yi (from the Container Parameters subtab of the Operation Parameters tab)	Yrm Yprod User-defined Yderm
Not Container-Related / Raw Material	Any	Yrm (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Yderm
Not Container Related / Product	Any	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Yderm
Not Container-Related / Neither Raw Material nor Product	Manufacturing	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Yderm
	Processing Use	Yrm (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Yderm

# Table B-13a. Conditional Default Values for Yderm for the EPA/OPPT 2-Hand Dermal Contact with Liquids Model

\*Non-default options for Yderm are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab. All default and non-default options for Yderm are available for both Output 1 and Output 2.

Source/Activity Type / Operation Mode	Batch Condition	Conditional ED Default (days of exposure/site-yr)	Non-default Options for ED
Container-Related / Continuous	Not applicable	Lesser of 250 or ODa (from Container Parameters subtab of the Operation Parameters tab)	OD (days/site-yr) User-defined ED
Container-Related / Batch	Any	Lesser of 250 or ODa (from Container Parameters subtab of the Operation Parameters tab)	Nby (bt/site-yr) OD (days/site-yr) User-defined ED
Not Container Related / Continuous	Not applicable	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	User-defined ED
Not Container-Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or Nby (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD User-defined ED
	Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby User-defined ED

## Table B-13b. Conditional Default Values for ED for the EPA/OPPT 2-Hand Dermal Contact with Liquids Model

\*Non-default options for ED are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab. All default and non-default options for ED are available for both Output 1 and Output 2.

## Key Rationale for Model

Dermal exposures to a chemical are estimated using standard assumptions documented in the references, and assume no use of controls or gloves to reduce exposures. For a given worker activity, this method assumes a specific surface area contacted by chemical and a specific surface density of that chemical to estimate a PDR using the model equations.

## References

US EPA/OPPT/CEB. Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991. (Equations 4-26)

US EPA Memo entitled Draft Guidance on LADDs and APDRs from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93.

US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.

## EPA/OPPT 2-Hand Dermal Immersion with Liquid Model

## **Model Description**

This model estimates dermal exposure to the chemical for 2-hand immersion in liquid containing the chemical.

## Sources/Activities That Use This Model as a Default

The EPA/OPPT 2-Hand Dermal Immersion in Liquids Model is the default for calculating worker dermal exposures to a liquid chemical while performing the following sources/activities:

- All sources/activities for <u>Automobile Spray Coating</u>
- Miscellaneous Sources/Activities Related to Liquid Processing

## EPA/OPPT 2-Hand Dermal Immersion in Liquids Model – Other Sources/Activities

The EPA/OPPT 2-Hand Dermal Immersion in Liquids Model may be an appropriate alternative to the default dermal model for the following sources/activities:

- All sources/activities for <u>Cleaning Liquid Residuals from Transport Containers/Vessels</u>
- All sources/activities for <u>Unloading Liquids from Transport Containers/Vessels</u>
- All sources/activities for Equipment Cleaning Losses of Liquids
- All sources/activities for <u>Sampling Liquids</u>
- Filter Media Changeout
- Coating Using Hand Held Spray Gun

## Potential Route / Form(s) of Exposure

Dermal contact / Liquid

#### **Equations**

Parameters	Description	Equation	Units
Dexp	Dermal potential dose rate	S x Qu x Yderm x FT	mg/day
NW	Total number of workers exposed	NWexp x NS	workers
LADD	Lifetime average daily dose	(Dexp x ED x EY)/(BW x ATc x 365 days/yr)	mg/kg-day
ADD	Average daily dose	(Dexp x ED x EY)/(BW x AT x 365 days/yr)	mg/kg-day
APDR	Acute potential dose rate	Dexp/BW	mg/kg-day

## **Model Input Parameters and Default Values**

The EPA/OPPT 2-Hand Dermal Immersion in Liquids Model default values for each of the input parameters are summarized in Table B-14.

Parameter	Description	Default Value(s)	Units
S	Surface area of contact (two hands) (constant)	1,070 (mean)	cm <sup>2</sup>
Qu	Quantity remaining on skin (constant)	Output 1: <u>Default:</u> 1.3 (low) <u>Non-default option:</u> 10.3 (high) Output 2: <u>Default:</u> 10.3 (high) <u>Non-default Option:</u> 1.3 (low)	mg/cm <sup>2</sup> -event
Yderm	Weight fraction of chemical in liquid (0 ≤ Yderm ≤ 1)	Defaults specified in Table B-14a	dimensionless
FT	Frequency of events (0 ≤ FT (integer)	1	events/worker-day
NWexp	Number of workers exposed while performing the activity	1	workers/site
NS	Number or sites	NS (from Mass Balance Parameters subtab of the Operation Parameters tab)	site(s)
ED	Days exposed per year (0 ≤ ED (integer) ≤ 365)	Defaults specified in Table B-14b	days/site-yr
EY	Years of occupational exposure (0 ≤ EY)	40	years
BW	Body weight (0 ≤ ATc)	70	kg
ATc	Averaging time over a lifetime (chronic) (0 ≤ ATc)	70	years
AT	Averaging time (EY ≤ AT ≤ ATc)	EY	years

## Table B-14. Input Parameters and Default Values for the EPA/OPPT 2-Hand Dermal Immersion in Liquids Model

You may elect to change any parameter from Table B-14 except S and Qu, which are constants. Clicking the *Type* column for each changeable parameter other than S, Qu, Yderm and ED contains only two options: ChemSTEER defaults from Table B-14 and User-defined. The conditional default and non-default options for Yderm and ED are presented in the tables below. Be sure to read the <u>ChemSTEER</u> <u>Estimation Methods and Models</u> topic for more information about changing model parameters.

NOTE on FT: Only one contact per day (FT = 1) is assumed because Qu, with few exceptions, is not expected to be significantly affected either by wiping excess from skin or by repeated contact(s) with additional chemical (i.e., wiping excess from the skin does not remove a significant fraction of the small layer of chemical adhering to the skin and additional contacts with the chemical do not add a significant fraction to the layer). Exceptions to this assumption may be considered for chemicals with high volatility and/ or with very high rates of absorption into the skin.

If you enter a User-defined FT and the value is greater than 1, ChemSTEER will display a warning message with the following text: "The value of FT should not exceed 1 unless the chemical assessed is

highly volatile or has a high rate of absorption. See the *Note on FT* in the User Guide topic for any dermal model for more information on this issue." After clicking "OK" you will be allowed to continue.

You may not change the defining model parameters, Qu and S, to be anything other than the defaults shown above. If you wish to model dermal exposures using your own data, choose the <u>US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.</u> User-Defined Dermal Model.

**NOTE:** It is assumed that the same number of workers dermally exposed to the chemical during the activity will also have an inhalation exposure (if an inhalation exposure is expected). If you update the number of workers exposed (NWexp), the NWexp for the corresponding output in the inhalation model, selected for the same activity, will be automatically updated with the entered value. For example, if you update NWexp for Output 2 in this model, NWexp for Output 2 in the inhalation model will be updated to the same value. The same is true if you update NWexp for Output 1.

## Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Settings for either Output 1 or Output 2 results are based on which Qu is selected for the corresponding output:

- Results using the low remaining quantity (Qu) are characterized as *Output 1* by default.
- Results using the high remaining quantity (Qu) are characterized as *High End* by default.

You may select an alternative characterization for either of the outputs at any time.

## **Default Model Basis**

The following default text is displayed in the Basis box on the View/Update Exposure Model Information screen:

"EPA/OPPT 2-Hand Dermal Immersion in Liquids Model."

Source/Activity Type / Material Named in Source/Activity Label	Operation Type	Conditional Yderm Default	Non-default Options for Yderm
Container-Related / Any	Any	Yi (from the Container Parameters subtab of the Operation Parameters tab)	Yrm Yprod User-defined Yderm
Not Container-Related / Raw Material	Any	Yrm (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Yderm
Not Container Related / Product	Any	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Yderm
Not Container-Related / Neither Raw Material nor Product	Manufacturing	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Yderm
	Processing Use	Yrm (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Yderm

# Table B-14a. Conditional Default Values for Yderm for the EPA/OPPT 2-Hand Dermal Immersion in Liquids Model

\*Non-default options for Yderm are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab. All default and non-default options for Yderm are available for both Output 1 and Output 2.

Source/Activity Type / Operation Mode	Batch Condition	Conditional ED Default (days of exposure/site-yr)	Non-default Options for ED
Container-Related / Continuous	Not applicable	Lesser of 250 or ODa (from Container Parameters subtab of the Operation Parameters tab)	OD (days/site-yr) User-defined ED
Container-Related / Batch	Any	Lesser of 250 or ODa (from Container Parameters subtab of the Operation Parameters tab)	Nby (bt/site-yr) OD (days/site-yr) User-defined ED
Not Container Related / Continuous	Not applicable	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	User-defined ED
Not Container-Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or Nby (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD User-defined ED
	Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby User-defined ED

## Table B-14b. Conditional Default Values for ED for the EPA/OPPT 2-Hand Dermal Immersion in Liquids Model

\*Non-default options for ED are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab. All default and non-default options for ED are available for both Output 1 and Output 2.

## Key Rationale for Model

Dermal exposures to a chemical are estimated using standard assumptions documented in the references, and assume no use of controls or gloves to reduce exposures. For a given worker activity, this method assumes a specific surface area contacted by chemical and a specific surface density of that chemical to estimate a PDR using the model equations.

## References

US EPA/OPPT/CEB. Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991. (Equations 4-26)

US EPA Memo entitled Draft Guidance on LADDs and APDRs from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93.

US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.

## EPA/OPPT Direct 2-Hand Dermal Contact with Solids Model

## **Model Description**

This model estimates dermal exposure to the chemical for direct 2-hand contact with solids containing the chemical.

## Sources/Activities That Use This Model as a Default

The EPA/OPPT Direct 2-Hand Dermal Contact with Solids Model is the default for calculating worker dermal exposures to a solid chemical while performing the following sources/activities:

- All sources/activities for <u>Cleaning Solid Residuals from Transport Containers/Vessels</u>
- All sources/activities for Loading Solids into Transport Containers/Vessels
- All sources/activities for <u>Unloading Solids from Transport Containers/Vessels</u>
- All sources/activities for <u>Sampling Solids</u>
- Equipment Cleaning Losses of Solids
- <u>Miscellaneous Sources/Activities Related to Solid Processing</u>
- Filter Media Changeout
- Grinding and Sanding

This model is not used as an alternative dermal exposure model for any other sources/activities.

## Potential Route / Form(s) of Exposure

Dermal contact / Solid

## Equations

Parameters	Description	Equation	Units
Dexp	Dermal potential dose rate	S x Qu x Yderm x FT	mg/day
NW	Total number of workers exposed	NWexp x NS	workers
LADD	Lifetime average daily dose	(Dexp x ED x EY)/(BW x ATc x 365 days/yr)	mg/kg-day
ADD	Average daily dose	(Dexp x ED x EY)/(BW x AT x 365 days/yr)	mg/kg-day
APDR	Acute potential dose rate	Dexp/BW	mg/kg-day

## **Model Input Parameters and Default Values**

The EPA/OPPT Direct 2-Hand Dermal Contact with Solids Model default values for each of the input parameters are summarized in Table B-15.

Parameter	Description	Default Value(s)	Units
S x Qu	Total amount of solids on skin	3,100 (high)	mg/event
Yderm	Weight fraction of chemical in liquid (0 ≤ Yderm ≤ 1)	Defaults specified in Table B-15a	dimensionless
FT	Frequency of events (0 ≤ FT (integer)	1	events/worker-day
NWexp	Number of workers exposed while performing the activity	1	workers/site
NS	Number or sites	NS (from Mass Balance Parameters subtab of the Operation Parameters tab)	site(s)
ED	Days exposed per year (0 ≤ ED (integer) ≤ 365)	Defaults specified in Table B-15b	days/site-yr
EY	Years of occupational exposure (0 ≤ EY)	40	years
BW	Body weight (0 ≤ ATc)	70	kg
ATc	Averaging time over a lifetime (chronic) (0 ≤ ATc)	70	years
AT	Averaging time (EY $\leq$ AT $\leq$ ATc)	EY	years

## Table B-15. Input Parameters and Default Values for the EPA/OPPT Direct 2-Hand Dermal Contact with Solids Model

You may elect to change any parameter from Table B-15 except (S x Qu), which are constants. Clicking the *Type* column for each changeable parameter other than (S x Qu), Yderm and ED contains only two options: ChemSTEER defaults from Table B-15 and User-defined. The conditional default and non-default options for Yderm and ED are presented in the tables below. Be sure to read the <u>ChemSTEER Estimation Methods and Models</u> topic for more information about changing model parameters.

NOTE on FT: Only one contact per day (FT = 1) is assumed because Qu, with few exceptions, is not expected to be significantly affected either by wiping excess from skin or by repeated contact(s) with additional chemical (i.e., wiping excess from the skin does not remove a significant fraction of the small layer of chemical adhering to the skin and additional contacts with the chemical do not add a significant fraction to the layer). Exceptions to this assumption may be considered for chemicals with high volatility and/ or with very high rates of absorption into the skin.

If you enter a User-defined FT and the value is greater than 1, ChemSTEER will display a warning message with the following text: "The value of FT should not exceed 1 unless the chemical assessed is highly volatile or has a high rate of absorption. See the *Note on FT* in the User Guide topic for any dermal model for more information on this issue." After clicking "OK" you will be allowed to continue.

You may not change the defining model parameter, (Qu x S), to be anything other than the default shown above. If you wish to model dermal exposures using your own data, choose the

<u>US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal</u> <u>Exposure, September 2013.</u> User-Defined Dermal Model.

NOTE: It is assumed that the same number of workers dermally exposed to the chemical during the activity will also have an inhalation exposure (if an inhalation exposure is expected). If you update the number of workers exposed (NWexp), the NWexp for the corresponding output in the inhalation model, selected for the same activity, will be automatically updated with the entered value. For example, if you update NWexp for Output 2 in this model, NWexp for Output 2 in the inhalation model will be updated to the same value. The same is true if you update NWexp for Output 1.

## Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default Characterization of Output 1 Results: *High End* Default Characterization of Output 2 Results: *High End* 

You may select an alternative characterization for either of the outputs at any time.

#### **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Exposure Model Information* screen:

"EPA/OPPT Direct 2-Hand Dermal Contact with Solids Model"

Source/Activity Type / Material Named in Source/Activity Label	Operation Type	Conditional Yderm Default	Non-default Options for Yderm
Container-Related / Any	Any	Yi (from the Container Parameters subtab of the Operation Parameters tab)	Yrm Yprod User-defined Yderm
Not Container-Related / Raw Material	Any	Yrm (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Yderm
Not Container Related / Product	Any	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Yderm
Not Container-Related / Neither Raw Material nor Product	Manufacturing	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Yderm
	Processing Use	Yrm (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Yderm

# Table B-15a. Conditional Default Values for Yderm for the EPA/OPPT Direct 2-Hand Dermal Contactwith Solids Model

\*Non-default options for Yderm are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab. All default and non-default options for Yderm are available for both Output 1 and Output 2.

Source/Activity Type / Operation Mode	Batch Condition	Conditional ED Default (days of exposure/site-yr)	Non-default Options for ED
Container-Related / Continuous	Not applicable	Lesser of 250 or ODa (from Container Parameters subtab of the Operation Parameters tab)	OD (days/site-yr) User-defined ED
Container-Related / Batch	Any	Lesser of 250 or ODa (from Container Parameters subtab of the Operation Parameters tab)	Nby (bt/site-yr) OD (days/site-yr) User-defined ED
Not Container Related / Continuous	Not applicable	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	User-defined ED
Not Container-Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or Nby (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD User-defined ED
	Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby User-defined ED

## Table B-15b. Conditional Default Values for ED for the EPA/OPPT Direct 2-Hand Dermal Contact with Solids Model

\*Non-default options for ED are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab. All default and non-default options for ED are available for both Output 1 and Output 2.

## Key Rationale for Model

Dermal exposures to a chemical are estimated using standard assumptions documented in the references, and assume no use of controls or gloves to reduce exposures. For a given worker activity, this method assumes a specific surface area contacted by chemical and a specific surface density of that chemical to estimate a PDR using the model equations.

## References

US EPA/OPPT/CEB. Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991. (Equations 4-26)

US EPA Memo entitled Draft Guidance on LADDs and APDRs from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93.

US EPA Memo entitled Revision to CEB's Method for Screening-Level Assessments of Dermal Exposure, June 2000.

## EPA/OPPT 2-Hand Dermal Contact with Container Surfaces Model

## **Model Description**

This model estimates dermal exposure to the chemical for 2-hand contact with surfaces on which solids containing the chemical are present.

## Sources/Activities That Use This Model as a Default

There are no sources/activities in ChemSTEER that use this model as a default for calculating worker dermal exposures to a chemical.

## EPA/OPPT 2-Hand Dermal Contact with Container Surfaces (Solids) Model – Sources/Activities

The EPA/OPPT 2-Hand Dermal Contact with Container Surfaces (solids) Model may be an appropriate means to calculate worker dermal exposures to a solid chemical while performing the following sources/activities:

- All sources/activities for <u>Cleaning Solid Residuals from Transport Containers/Vessels</u>
- All sources/activities for <u>Unloading Solids from Transport Containers/Vessels</u>
- All sources/activities for <u>Sampling Solids</u>
- Equipment Cleaning Losses of Solids
- Miscellaneous Sources/Activities Related to Solid Processing
- Filter Media Changeout
- Grinding and Sanding

## Potential Route / Form(s) of Exposure

Dermal contact / Solid

## Equations

Parameters	Description	Equation	Units
Dexp	Dermal potential dose rate	S x Qu x Yderm x FT	mg/day
NW	Total number of workers exposed	NWexp x NS	workers
LADD	Lifetime average daily dose	(Dexp x ED x EY)/(BW x ATc x 365 days/yr)	mg/kg-day
ADD	Average daily dose	(Dexp x ED x EY)/(BW x AT x 365 days/yr)	mg/kg-day
APDR	Acute potential dose rate	Dexp/BW	mg/kg-day

## **Model Input Parameters and Default Values**

The EPA/OPPT 2-Hand Dermal Contact with Container Surfaces (Solids) Model default values for each of the input parameters are summarized in Table B-16.

Parameter	Description	Default Value(s)	Units
S x Qu	Total amount of solids on skin	1,100 (high)	mg/event
Yderm	Weight fraction of chemical in liquid (0 ≤ Yderm ≤ 1)	Defaults specified in Table B-16a	dimensionless
FT	Frequency of events (0 ≤ FT (integer)	1	events/worker-day
NWexp	Number of workers exposed while performing the activity	1	workers/site
NS	Number or sites	NS (from Mass Balance Parameters subtab of the Operation Parameters tab)	site(s)
ED	Days exposed per year (0 ≤ ED (integer) ≤ 365)	Defaults specified in Table B-16b	days/site-yr
EY	Years of occupational exposure (0 ≤ EY)	40	years
BW	Body weight (0 ≤ ATc)	70	kg
АТс	Averaging time over a lifetime (chronic) (0 ≤ ATc)	70	years
AT	Averaging time (EY $\leq$ AT $\leq$ ATc)	EY	years

## Table B-16. Input Parameters and Default Values for the EPA/OPPT 2-Hand Dermal Contact with Container Surfaces (Solids) Model

You may elect to change any parameter from Table B-16 except (S x Qu), which is a constant. Clicking the *Type* column for each changeable parameter other than (S x Qu), Yderm and ED contains only two options: ChemSTEER defaults from Table B-16 and User-defined. The conditional default and non-default options for Yderm and ED are presented in the tables below. Be sure to read the <u>ChemSTEER Estimation Methods and Models</u> topic for more information about changing model parameters.

NOTE on FT: Only one contact per day (FT = 1) is assumed because Qu, with few exceptions, is not expected to be significantly affected either by wiping excess from skin or by repeated contact(s) with additional chemical (i.e., wiping excess from the skin does not remove a significant fraction of the small layer of chemical adhering to the skin and additional contacts with the chemical do not add a significant fraction to the layer). Exceptions to this assumption may be considered for chemicals with high volatility and/ or with very high rates of absorption into the skin.

If you enter a User-defined FT and the value is greater than 1, ChemSTEER will display a warning message with the following text: "The value of FT should not exceed 1 unless the chemical assessed is highly volatile or has a high rate of absorption. See the *Note on FT* in the User Guide topic for any dermal model for more information on this issue." After clicking "OK" you will be allowed to continue.

You may not change the defining model parameter, (Qu x S), to be anything other than the default shown above. If you wish to model dermal exposures using your own data, choose the <u>US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.</u>

## **User-Defined Dermal Model.**

NOTE: It is assumed that the same number of workers dermally exposed to the chemical during the activity will also have an inhalation exposure (if an inhalation exposure is expected). If you update the number of workers exposed (NWexp), the NWexp for the corresponding output in the inhalation model, selected for the same activity, will be automatically updated with the entered value. For example, if you update NWexp for Output 2 in this model, NWexp for Output 2 in the inhalation model will be updated to the same value. The same is true if you update NWexp for Output 1.

## Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Disabled* Enable Model Parameters for Output 2: *Enabled* 

Default Characterization of Output 1 Results: *High End* Default Characterization of Output 2 Results: *High End* 

You may select an alternative characterization for either of the outputs at any time.

## **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Exposure Model Information* screen:

"EPA/OPPT 2-Hand Dermal Contact with Container Surfaces (Solids) Model"

Source/Activity Type / Material Named in Source/Activity Label	Operation Type	Conditional Yderm Default	Non-default Options for Yderm
Container-Related / Any	Any	Yi (from the Container Parameters subtab of the Operation Parameters tab)	Yrm Yprod User-defined Yderm
Not Container-Related / Raw Material	Any	Yrm (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Yderm
Not Container Related / Product	Any	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Yderm
Not Container-Related / Neither Raw Material nor Product	Manufacturing	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Yderm
	Processing Use	Yrm (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Yderm

# Table B-16a. Conditional Default Values for Yderm for the EPA/OPPT 2-Hand Dermal Contact with Container Surfaces (Solids) Model

\*Non-default options for Yderm are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab. All default and non-default options for Yderm are available for both Output 1 and Output 2.

Source/Activity Type / Operation Mode	Batch Condition	Conditional ED Default (days of exposure/site-yr)	Non-default Options for ED
Container-Related / Continuous	Not applicable	Lesser of 250 or ODa (from Container Parameters subtab of the Operation Parameters tab)	OD (days/site-yr) User-defined ED
Container-Related / Batch	Any	Lesser of 250 or ODa (from Container Parameters subtab of the Operation Parameters tab)	Nby (bt/site-yr) OD (days/site-yr) User-defined ED
Not Container Related / Continuous	Not applicable	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	User-defined ED
Not Container-Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or Nby (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD User-defined ED
	Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby User-defined ED

# Table B-16b. Conditional Default Values for ED for the EPA/OPPT 2-Hand Dermal Contact with Container Surfaces (Solids) Model

\*Non-default options for ED are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab. All default and non-default options for ED are available for both Output 1 and Output 2.

## Key Rationale for Model

Dermal exposures to a chemical are estimated using standard assumptions documented in the references, and assume no use of controls or gloves to reduce exposures. For a given worker activity, this method assumes a specific surface area contacted by chemical and a specific surface density of that chemical to estimate a PDR using the model equations.

## References

US EPA/OPPT/CEB. Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991. (Equations 4-26)

US EPA Memo entitled Draft Guidance on LADDs and APDRs from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93.

US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.

## User-Defined Dermal Model

## **Model Description**

This model estimates the amount of chemical potentially contacted to a worker's skin during an activity. Estimation of the exposure amount is based on user-input values of skin surface area contacted and amount per area contacted.

## Sources/Activities That Use This Model as a Default

There are no sources/activities in ChemSTEER that use this model as a default for calculating worker dermal exposures to a chemical.

This model is appropriate to use as an alternative dermal model for <u>all</u> other ChemSTEER sources/activities (except the *Recirculating Water-Cooling Tower Additive Releases* source/activity).

## Potential Route / Form(s) of Exposure

Dermal contact / Liquid or solid

## Equations

Parameters	Description	Equation	Units
Dexp	Dermal potential dose rate	S x Qu x Yderm x FT	mg/day
NW	Total number of workers exposed	NWexp x NS	workers
LADD	Lifetime average daily dose	(Dexp x ED x EY)/(BW x ATc x 365 days/yr)	mg/kg-day
ADD	Average daily dose	(Dexp x ED x EY)/(BW x AT x 365 days/yr)	mg/kg-day
APDR	Acute potential dose rate	Dexp/BW	mg/kg-day

## **Model Input Parameters and Default Values**

The User-Defined Dermal Model default values for each of the input parameters are summarized in Table B-17.

Parameter	Description	Default Value(s)	Units
S	Surface area of contact (one hands) (constant)	<i>Output 1:</i> <u>Default:</u> 535 (low, one hand) <u>Non-default Options:</u> 1,070 (high, two hands) and User-defined S	cm <sup>2</sup>
		<i>Output 2:</i> <u>Default:</u> 1,070 (high, two hands) <u>Non-default Options:</u> 535 (low, one hand) and User-defined S	
Qu	Quantity remaining on skin (constant)	<i>Output 1:</i> <u>Default:</u> 0.7 (low) <u>Non-default option:</u> 2.1 (high) and User-defined Qu	mg/cm <sup>2</sup> -event
		<i>Output 2:</i> <u>Default:</u> 2.1 (high) <u>Non-default Option:</u> 0.7 (low) and User-defined Qu	
Yderm	Weight fraction of chemical in liquid (0 ≤ Yderm ≤ 1)	Defaults specified in Table B-17a	dimensionless
FT	Frequency of events (0 ≤ FT (integer)	1	events/worker-day
NWexp	Number of workers exposed while performing the activity	1	workers/site
NS	Number or sites	NS (from Mass Balance Parameters subtab of the Operation Parameters tab)	site(s)
ED	Days exposed per year (0 ≤ ED (integer) ≤ 365)	Defaults specified in Table B-17b	days/site-yr
EY	Years of occupational exposure (0 ≤ EY)	40	years
BW	Body weight (0 ≤ ATc)	70	kg
ATc	Averaging time over a lifetime (chronic) (0 ≤ ATc)	70	years
AT	Averaging time (EY $\leq$ AT $\leq$ ATc)	EY	years

Table B-17. Input Parameters and Default Values for the User-Defined Dermal Model

You may elect to change any parameter from Table B-17. Clicking the *Type* column for each changeable parameter other than Yderm and ED contains only two options: ChemSTEER defaults from Table B-17 and User-defined. You may elect to enter values for S and/or Qu in this exposure model. Alternatively, you may select one of the default values shown in Table B-17. The conditional default and non-default options for Yderm and ED are presented in the tables below. Be sure to read the <u>ChemSTEER Estimation Methods and Models</u> topic for more information about changing model parameters.

NOTE on FT: Only one contact per day (FT = 1) is assumed because Qu, with few exceptions, is not expected to be significantly affected either by wiping excess from skin or by repeated

contact(s) with additional chemical (i.e., wiping excess from the skin does not remove a significant fraction of the small layer of chemical adhering to the skin and additional contacts with the chemical do not add a significant fraction to the layer). Exceptions to this assumption may be considered for chemicals with high volatility and/ or with very high rates of absorption into the skin.

If you enter a User-defined FT and the value is greater than 1, ChemSTEER will display a warning message with the following text:

"The value of FT should not exceed 1 unless the chemical assessed is highly volatile or has a high rate of absorption. See the Note on FT in the User Guide topic for any dermal model for more information on this issue."

After clicking "OK" you will be allowed to continue.

NOTE: It is assumed that the same number of workers dermally exposed to the chemical during the activity will also have an inhalation exposure (if an inhalation exposure is expected). If you update the number of workers exposed (NWexp), the NWexp for the corresponding output in the inhalation model, selected for the same activity, will be automatically updated with the entered value. For example, if you update NWexp for Output 2 in this model, NWexp for Output 2 in the inhalation model will be updated to the same value. The same is true if you update NWexp for Output 1.

## Default Parameter Value Switch Settings and Results Characterization

Enable Model Parameters for Output 1: *Enabled* Enable Model Parameters for Output 2: *Enabled* 

Default Characterization of Output 1 Results: *Output 1* Default Characterization of Output 2 Results: *Output 2* 

You may select an alternative characterization for either of the outputs at any time.

## **Default Model Basis**

The following default text is displayed in the *Basis* box on the *View/Update Exposure Model Information* screen:

"User-Defined Dermal Model"
Source/Activity Type / Material Named in Source/Activity Label	Operation Type	Conditional Yderm Default	Non-default Options for Yderm
Container-Related / Any	Any	Yi (from the Container Parameters subtab of the Operation Parameters tab)	Yrm Yprod User-defined Yderm
Not Container-Related / Raw Material	Any	Yrm (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Yderm
Not Container Related / Product	Any	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Yderm
Not Container-Related / Neither Raw Material nor Product	Manufacturing	Yprod (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yrm User-defined Yderm
	Processing Use	Yrm (from Mass Balance Parameters subtab of the Operation Parameters tab)	Yprod User-defined Yderm

|--|

\*Non-default options for Yderm are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab. All default and non-default options for Yderm are available for both Output 1 and Output 2.

Source/Activity Type / Operation Mode	Batch Condition	Conditional ED Default (days of exposure/site-yr)	Non-default Options for ED
Container-Related / Continuous	Not applicable	Lesser of 250 or ODa (from Container Parameters subtab of the Operation Parameters tab)	OD (days/site-yr) User-defined ED
Container-Related / Batch	Any	Lesser of 250 or ODa (from Container Parameters subtab of the Operation Parameters tab)	Nby (bt/site-yr) OD (days/site-yr) User-defined ED
Not Container Related / Continuous	Not applicable	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	User-defined ED
Not Container-Related / Batch	Number of batches per day (Nbd) < 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or Nby (from Mass Balance Parameters subtab of the Operation Parameters tab)	OD User-defined ED
	Number of batches per day (Nbd) ≥ 1 (from Mass Balance Parameters subtab of the Operation Parameters tab)	Lesser of 250 or OD (from Mass Balance Parameters subtab of the Operation Parameters tab)	Nby User-defined ED

Table B-17b. Conditional Default	Values for ED for the	User-Defined Dermal Model

\*Non-default options for ED are available by clicking in the *Type* column in the View/Update Exposure Model Information screen in the Exposures tab. All default and non-default options for ED are available for both Output 1 and Output 2.

## Key Rationale for Model

For a given worker activity, this method assumes a user-defined surface area contacted by chemical and a user-defined surface density of that chemical to estimate a Dexp using the model equations.

## References

US EPA/OPPT/CEB. Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991. (Equations 4-26)

US EPA Memo entitled Draft Guidance on LADDs and APDRs from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93.

US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.

# Models for Calculating Exposures to Liquids

## Exposures as a Result of Evaporation

The following models may be selected for sources/activities that result in inhalation exposure to evaporation:

- EPA/OPPT Mass Balance Inhalation Model
- OSHA PEL-Limiting Model for Substance-Specific Vapors
- User-Defined Inhalation Model

## Exposures During Container Filling (Vapor Displacement)

The following models may be selected for sources/activities that result in inhalation exposure during container filling:

- EPA/OPPT Mass Balance Inhalation Model
- OSHA PEL-Limiting Model for Substance-Specific Vapors
- User-Defined Inhalation Model

## *Exposures to Mists*

The following models may be selected for sources/activities that result in inhalation exposure to mists:

- OSHA PEL-Limiting Model for Substance-Specific Particulates
- OSHA Total PNOR PEL-Limiting Model
- OSHA Respirable PNOR PEL-Limiting Model
- EPA/OPPT Automobile OEM Spray Coating Inhalation Exposure Model
- EPA/OPPT Automobile Refinish Spray Coating Inhalation Exposure Model
- EPA/OPPT Automobile Spray Coating Inhalation Exposure Model
- EPA/OPPT UV Roll Coating Inhalation Model
- <u>User-Defined Inhalation Model</u>

## *Exposures from Touching Liquid Chemicals and/or Wet Surfaces*

The following models may be selected for sources/activities that result in dermal exposure from touching liquid chemicals and/or wet surfaces:

- EPA/OPPT 1-Hand Dermal Contact with Liquid Model
- EPA/OPPT 2-Hand Dermal Contact with Liquid Model

# US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal Exposure, September 2013.

EPA/OPPT 2-Hand Dermal Immersion with Liquid Model

<u>US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal</u> <u>Exposure, September 2013.</u> • User-Defined Dermal Model

# Models for Calculating Exposures to Solids

## Exposures to Dusts

The following models may be selected for sources/activities that result in inhalation exposure to dusts:

- EPA/OPPT Small Volume Solids Handling Inhalation Model
- OSHA PEL-Limiting Model for Substance-Specific Particulates
- OSHA Total PNOR PEL-Limiting Model
- OSHA Respirable PNOR PEL-Limiting Model
- User-Defined Inhalation Model

# Exposures from Touching Solid Chemicals and/or Dusty Surfaces

The following models may be selected for sources/activities that result in dermal exposure from touching solid chemicals and/or dusty surfaces:

- EPA/OPPT Direct 2-Hand Dermal Contact with Solids Model
- EPA/OPPT 2-Hand Dermal Contact with Container Surfaces Model

<u>US EPA Memo entitled Updating CEB's Method for Screening-Level Assessments of Dermal</u> <u>Exposure, September 2013.</u>

User-Defined Dermal Model

## Models for Calculating Exposures Based on Exposure Limits

The following models may be selected to calculate exposures based on exposure limits:

- OSHA PEL-Limiting Model for Substance-Specific Particulates
- OSHA PEL-Limiting Model for Substance-Specific Vapors
- OSHA Total PNOR PEL-Limiting Model
- OSHA Respirable PNOR PEL-Limiting Model

# **Definitions and Terms**

# **Abbreviations**

The following list is a <u>draft</u> list of all parameter abbreviations and other key assessment-related abbreviations used in ChemSTEER (as of September 30, 2013) and is in alphabetical order. In future ChemSTEER User Guides, the definitions will be refined and standardized.

A [area (cm2)] - area of liquid pool. <u>EPA/OPPT Mass Transfer Coefficient Model</u>, <u>EPA/OPPT</u> <u>Penetration Model</u>

ADD [average daily dose (mg/kg-day)] - output from all exposure models in ChemSTEER. Same as LADD except uses AT rather than ATc. LADD from pages 3 and 4 of US EPA Memo entitled <u>Draft</u> <u>Guidance on LADDs and APDRs</u> from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93

**ADMUaddtv [average daily mass of bath additive (kg/site-day)]** - Averaged daily mass of the bath additive used to replace intermittent losses from bath changes and daily losses from rinsing parts from <u>Electroplating Bath Additive Use</u> operation.

ADMUchem [average daily mass of chemical in bath additive used to replace intermittent losses from bath changes and daily losses from rinsing parts (kg/site-day)] - Averaged daily mass of chemical in the bath additive used to replace intermittent losses from bath changes and daily losses from rinsing parts. <u>Electroplating Bath Additive Use</u>.

**AH [amount of material handled (kg/day)]** - input to an inhalation model, amount (mass) of solids/ powder containing the chemical handled by a worker in an activity (limited to up to 54 kg/ worker/ shift). <u>EPA/OPPT Small Volume Solids Handling Inhalation Model</u>

Amt [amount of chemical to which a loss fraction (LF) is applied (kg/site-day)] - input for many release models. This amount is often equal to a key mass or container-related parameter for the operation such as the mass of chemical per batch or per container. EPA/OPPT Bulk Transport Residual Model, EPA/OPPT Drum Residual Model, EPA/OPPT Multiple Process Vessel Residual Model, EPA/OPPT Single Vessel Residual Model, EPA/OPPT Small Container Residual Model, EPA/OPPT Solid Residuals in Transport Containers Model, EPA/OPPT Water Saturation Loss Model, User-Defined Loss Rate Model.

**APDR [average potential dose rate (mg/kg-day)]** - output from all exposure models in ChemSTEER from pages 3 and 4 of US EPA Memo entitled <u>Draft Guidance on LADDs and APDRs</u> from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93

**AR [annual release rate of assessed chemical (kg/year)]** - output from all release models in ChemSTEER; calculated by the equation AR = DR × Freq × NS, AR is for all sites combined

**AT [averaging time (years)]** - input to all exposure models to calculate ADD; default of EY. US EPA Memo entitled <u>Draft Guidance on LADDs and APDRs</u> from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93

**ATc [averaging time - chronic (years)]** - input to all exposure models to calculate LADD; default of 70 assumed as a reasonably conservative value from pages 5 and 6 default values list of US EPA Memo entitled <u>Draft Guidance on LADDs and APDRs</u> from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93

## atm [atmospheres] - unit of measure of pressure

AVPlow [low end of adjusted vapor pressure range (torr)] - bounding adjusted vapor pressure value, below which ChemSTEER will not default to using vapor generation models for calculating releases to air from and inhalation exposures to liquid materials; refer to the *Preferences* menu topic, <u>Vapor Model Activation</u>

**AVPhigh [high end of adjusted vapor pressure range (torr)]** - bounding adjusted vapor pressure value, above which ChemSTEER will not default to using any of the vapor generation models for calculating releases to air from and inhalation exposures to liquid materials; refer to the *Preferences* menu topic, <u>Vapor Model Activation</u>

**AVPprod [adjusted vapor pressure of product material (torr)]** - applied to the preferred AVPrange to determine whether the vapor generation release and exposure models are applicable for the operation; ChemSTEER will only execute these models by default when AVPprod is within AVPrange; refer to the <u>Vapor Model Activation</u> topic

**AVPrange [preferred range in adjusted vapor pressure values (torr)]** - bounded by AVPlow and AVPhigh; if a liquid material's adjusted vapor pressure (AVPrm or AVPprod) is within the range, ChemSTEER will utilize default vapor generation models for calculating releases to air and worker inhalation exposures; refer to the *Preferences* menu topic, <u>Vapor Model Activation</u>

AVPraw [adjusted vapor pressure of raw material (torr)] - applied to the preferred AVPrange to determine whether the vapor generation release and exposure models are applicable for the operation; ChemSTEER will only execute these models by default when AVPrmz is within AVPrange; refer to the <u>Operation Parameters Tab  $\rightarrow$  Shared Parameters/Factors Subtab</u> topic

**b** [volumetric inhalation rate (m3/hour)] - input to most inhalation exposure models; default of 1.25 assumed as a reasonably conservative value (slightly above "light work" rate) based on Table 4-1 of Chapter 4 of <u>Chemical Engineering Branch Manual for the Preparation of Engineering Assessments</u>, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991

**BMIchem [batch mass input of chemical (kg/site-btc)]** - input or output for batch operations in the *Mass Balance Parameters* subtab; input, either alone or in combination with other batch parameters, as option(s) for Amt for release models using loss fractions (LF) and for exposure models using amount handled (AH). <u>EPA/OPPT Bulk Transport Residual Model</u>, <u>EPA/OPPT Drum Residual Model</u>, <u>EPA/OPPT Multiple Process Vessel Residual Model</u>, <u>EPA/OPPT Single Vessel Residual Model</u>, <u>EPA/OPPT Small Container Residual Model</u>, <u>EPA/OPPT Solid Residuals in Transport Containers Model</u>, <u>EPA/OPPT</u> <u>Water Saturation Loss Model</u>, <u>User-Defined Loss Rate Model</u>; <u>EPA/OPPT Small Volume Solids Handling</u> <u>Inhalation Model</u>

**BMIrm [batch mass input of raw material (kg/site-btc)]** - input or output for batch operations in the *Mass Balance Parameters* subtab; input, either alone or in combination with other batch parameters, to equations used in *Container Parameter* subtab value calculations

**BMOchem [batch mass output of chemical (kg/site-btc)]** - input or output for batch operations in the Mass Balance Parameters subtab; input, either alone or in combination with other batch parameters, as option(s) for Amt for release models using loss fractions (LF) and for exposure models using amount handled (AH). <u>EPA/OPPT Bulk Transport Residual Model</u>, <u>EPA/OPPT Drum Residual Model</u>, <u>EPA/OPPT Multiple Process Vessel Residual Model</u>, <u>EPA/OPPT Single Vessel Residual Model</u>, <u>EPA/OPPT Small Container Residual Model</u>, <u>EPA/OPPT Solid Residuals in Transport Containers Model</u>, <u>EPA/OPPT</u> <u>Water Saturation Loss Model</u>, User-Defined Loss Rate Model; <u>EPA/OPPT Small Volume Solids Handling</u> <u>Inhalation Model</u> **BMOprod [batch mass output of product (kg/site-btc)]** - input or output for batch operations in the *Mass Balance Parameters* subtab; input, either alone or in combination with other batch parameters, to equations used in *Container Parameter* subtab value calculations

**BW [body weight (kg)]** - input to all exposure models to calculate LADD, ADD, ADPR; default of 70 assumed as a reasonably conservative value from pages 5 and 6 default values list of US EPA Memo entitled <u>Draft Guidance on LADDs and APDRs</u> from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93

C (or °C) [degrees Celsius] - unit of measure of temperature

**CF** [correction factor (dimensionless)] - a factor that the user may use to adjust the amount released to account for: a) multiples of an amount (Amt) of water (e.g., for multiple washings); b) known or estimated correction of the water solubility of the chemical; and/or c) other corrections; <u>EPA/OPPT</u> Water Saturation Loss Model

**Cm** [mass concentration of chemical in air (mg/m3)] - input and/ or output from all inhalation exposure models; <u>EPA/OPPT Small Volume Solids Handling Inhalation Model</u>, <u>EPA/OPPT Mass Balance</u> <u>Inhalation Model</u>, <u>OSHA PEL-Limiting Model for Substance-Specific Particulates</u>, <u>OSHA PEL-Limiting</u> <u>Model for Substance-Specific Vapors</u>, <u>OSHA Total PNOR PEL-Limiting Model</u>, <u>OSHA Respirable PNOR PEL-Limiting Model</u>, <u>User-Defined Inhalation Model</u>

cm2 [square centimeters] - unit of measure of surface area

**Cv** [volumetric concentration of chemical in air (ppm)] - input and/ or output from all vapor inhalation exposure models; <u>EPA/OPPT Mass Balance Inhalation Model</u>, <u>OSHA PEL-Limiting Model for</u> <u>Substance-Specific Vapors</u>, <u>User-Defined Inhalation Model</u>

**Cvk** [volumetric vapor concentration of the chemical with an OSHA PEL in air (ppm)] - input to one inhalation exposure model. <u>OSHA PEL-Limiting Model for Substance-Specific Vapors</u>

**d** [diameter of opening or exposed pool of liquid (cm)] - input to release models that estimate vapor generation from open liquid pools. <u>EPA/OPPT Mass Transfer Coefficient Model</u>, <u>EPA/OPPT</u> <u>Penetration Model</u>

Dbath: Density of the electroplating bath (kg/liter). <u>Electroplating Bath Additive Use</u> operation.

**Dchem [density of the pure chemical (kg/L)]** - input for making volume-to-mass conversions in equations used in *Container Parameter* subtab value calculations

**Dexp [Dermal potential dose rate of the assessed chemical (mg/day)]** - output from all dermal exposure models in ChemSTEER; input to all dermal exposure models to calculate LADD, ADPR

**Di [density of material handled in a particular activity (kg/L)]** - input for making volume-tomass conversions in equations used in *Container Parameter* subtab value calculations

DMIchem [daily mass input of chemical (kg/site-day)] - input or output for continuous operations in the *Mass Balance Parameters* subtab; input, either alone or in combination with other batch parameters, as option(s) for Amt for release models using loss fractions (LF) and for exposure models using amount handled (AH). <u>EPA/OPPT Bulk Transport Residual Model</u>, <u>EPA/OPPT Drum Residual Model</u>, <u>EPA/OPPT Multiple Process Vessel Residual Model</u>, <u>EPA/OPPT Single Vessel Residual Model</u>, <u>EPA/OPPT Small Container Residual Model</u>, <u>EPA/OPPT Solid Residuals in Transport Containers Model</u>, <u>EPA/OPPT Water Saturation Loss Model</u>, User-Defined Loss Rate Model; <u>EPA/OPPT Small Volume Solids Handling Inhalation Model</u>

**DMIppaint [daily mass input of purchased paint (kg/site-day)]** - mass balance input parameter for the <u>Automobile Refinish Spray Coating Application</u> operation; input, either alone or in combination with other parameters, to the equations used in Container Parameters subtab calculations

**DMIrm [daily mass input of raw material (kg/site-day)]** - input or output for continuous operations in the *Mass Balance Parameters* subtab; input, either alone or in combination with other batch parameters, to equations used in *Container Parameter* subtab value calculations

DMOchem [daily mass output of chemical (kg/site-day)] - input or output for continuous operations in the *Mass Balance Parameters* subtab; input, either alone or in combination with other batch parameters, as option(s) for Amt for release models using loss fractions (LF) and for exposure models using amount handled (AH). <u>EPA/OPPT Bulk Transport Residual Model</u>, <u>EPA/OPPT Drum Residual Model</u>, <u>EPA/OPPT Multiple Process Vessel Residual Model</u>, <u>EPA/OPPT Single Vessel Residual Model</u>, <u>EPA/OPPT Small Container Residual Model</u>, <u>EPA/OPPT Solid Residuals in Transport Containers Model</u>, <u>EPA/OPPT Water Saturation Loss Model</u>, User-Defined Loss Rate Model; <u>EPA/OPPT Small Volume Solids Handling Inhalation Model</u>

**DMOprod [daily mass output of product (kg/site-day)]** - input or output for continuous operations in the *Mass Balance Parameters* subtab; input, either alone or in combination with other batch parameters, to equations used in *Container Parameter* subtab value calculations

**DMP [default model processing]** - function in ChemSTEER that adds default models to each source/activity, based on the conditions in the assessment

DMUchem [daily mass of chemical used (kg/site-day)] - input or output for the Automobile OEM Spray Coating Application and the Automobile Refinish Spray Coating Application operations in the Mass Balance Parameters subtab (DMUchem is a non-default for the Auto Refinish Spray Coating operation); input, either alone or in combination with other batch parameters, as option(s) for Amt for release models using loss fractions (LF) and for exposure models using amount handled (AH). EPA/OPPT Bulk Transport Residual Model, EPA/OPPT Drum Residual Model, EPA/OPPT Multiple Process Vessel Residual Model, EPA/OPPT Single Vessel Residual Model, EPA/OPPT Small Container Residual Model, EPA/OPPT Solid Residuals in Transport Containers Model, EPA/OPPT Water Saturation Loss Model, User-Defined Loss Rate Model; EPA/OPPT Small Volume Solids Handling Inhalation Model

**DMUfpaint [daily mass of formulated paint used (kg/site-day)]** - input or output for the <u>Automobile Refinish Spray Coating Application</u> operation in the Mass Balance Parameters subtab; only used in cases where the user elects an effluent basis for the operation Mass Balance Parameter calculations (this is the non-default option for this operation)

**DMUpaint [daily mass of paint used (kg/site-day)]** - input or output for the <u>Automobile OEM</u> <u>Spray Coating Application</u> operation in the Mass Balance Parameters subtab

**Dppaint [density of purchased paint (kg/L)]** - mass balance input parameter for making volumeto-mass conversions in the <u>Automobile Refinish Spray Coating Application</u> operation; used with DVIppaint to calculate DMIppaint

**Dprod [density of product material (kg/L)]** - input for making volume-to-mass conversions in equations used in *Container Parameter* subtab value calculations

**DR** [daily release rate (kg/site-day)] - model output for every release model in ChemSTEER; calculated by the relevant model equation

Drinse [density of the electroplating rinse (kg/liter)] <u>Electroplating Bath Additive Use</u> operation.

**Drm [density of raw material (kg/L)]** - input for making volume-to-mass conversions in equations used in *Container Parameter* subtab value calculations

**DVIppaint [daily volume of purchased paint used (liters/site-day)]** - input to the <u>Automobile</u> <u>Refinish Spray Coating Application</u> operation in the Mass Balance Parameters subtab; input with Dppaint to calculate DMIppaint

DVrinse: [daily volume of rinse water generated per site (gallons/site-day)] <u>Electroplating Bath</u> <u>Additive Use</u> operation.

ED [days exposed per year (days/site-year)] - input and output from all exposure models

**EF [exposure factor (mg/kg)]** - mg of solid material inhaled per kg handled; <u>EPA/OPPT Small</u> <u>Volume Solids Handling Inhalation Model</u>

**EPVop [estimated PVop for iterative calculation sequences]**. <u>Electroplating Bath Additive Use</u> operation.

**EY [years of occupational exposure (years)]** - input to all exposure models in ChemSTEER; default of 40 assumed as a reasonably conservative value from pages 5 and 6 of US EPA Memo entitled <u>Draft Guidance on LADDs and APDRs</u> from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93

**f** [saturation factor (dimensionless)] - input to release models in ChemSTEER that estimate vapor generation from vapor displacement, such as filling containers with liquids. EPA/OAQPS AP-42 Loading Model

**fc [fraction of PVop shipped in a particular container (dimensionless)]** - input to equations used in *Container Parameter* subtab value calculations

Percent of PV [PERCENT of {total} production volume (PV) associated with a particular operation (dimensionless)] - "Percent of PV" x PV / 100 = PVop (see Operation, <u>Operations Tab</u>  $\rightarrow$  <u>Relationships Subtab</u>)

Freq [frequency of release (days/site-yr)] - input and output from all release models

**Freqbath [frequency of bath changes per year (changes/bath/yr)].** <u>Electroplating Bath Additive</u> <u>Use</u> operation.

FT [frequency of dermal events (events/day)] - input to all dermal exposure models

g [grams] - unit of measure of mass

**G** [vapor generation rate of the assessed chemical (g/s, grams/second)] - input or output from all release models that estimate vapor generation. <u>EPA/OAQPS AP-42 Loading Model</u>, <u>EPA/OPPT Mass</u> <u>Transfer Coefficient Model</u>, <u>EPA/OPPT Penetration Model</u>, <u>User-Defined Vapor Generation Rate Model</u>

h [exposure duration (hrs/day)] - input or output from equations used in *Container Parameter* subtab value calculations; input to all inhalation exposure models <u>EXCEPT</u> *EPA/OPPT Small Volume Handling Model*, which does not have a time factor. <u>EPA/OPPT Mass Balance Inhalation Model</u>, <u>OSHA</u> <u>PEL-Limiting Model for Substance-Specific Particulates</u>, <u>OSHA PEL-Limiting Model for Substance-Specific</u> <u>Vapors</u>, <u>OSHA Total PNOR PEL-Limiting Model</u>, <u>OSHA Respirable PNOR PEL-Limiting Model</u>, <u>User-Defined</u> <u>Inhalation Model</u>

**HB** [hours per batch (hrs/btc)] - input or output for batch operations in the *Mass Balance Parameters* subtab

hr [hours] - unit of measure of time

**i** [activity designator] - indicates that the accompanying parameter may have a value that is particular to the source/activity being assessed

I [inhalation potential dose rate of the assessed chemical (mg/day)] - output from all inhalation exposure models in ChemSTEER; input to all inhalation exposure models to calculate LADD, ADD, ADPR

**IRER [Initial Review Engineering Report]** – a specially formatted EPA report for internal use for summarizing estimates of workplace (operation) releases and exposures in a particular assessment. <u>IRER</u> Format Details

K [degrees Kelvin] - unit of measure of temperature

k [mixing factor (dimensionless)] - used by the EPA/OPPT Mass Balance Inhalation Model

KCk [mass concentration of total or total respirable particulate in the air (mg/m3)] - input to all OSHA PEL particulate-related inhalation exposure models. <u>OSHA PEL-Limiting Model for Substance-</u> <u>Specific Particulates</u>, <u>OSHA Total PNOR PEL-Limiting Model</u>, <u>OSHA Respirable PNOR PEL-Limiting Model</u>

Kg [kilograms] - unit of measure of mass

L [liters] - unit of measure of volume

**LADD [lifetime average daily dose (mg/kg-day)]** - output from all exposure models in ChemSTEER from pages 3 and 4 of US EPA Memo entitled <u>Draft Guidance on LADDs and APDRs</u> from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93

LF [loss fraction (dimensionless) applied to a given amount (Amt) of chemical] - input to many release models. This loss is often based on data or another assumption and then multiplied by a given amount (mass) of chemical per batch or per container. <u>EPA/OPPT Bulk Transport Residual Model</u>, <u>EPA/OPPT Drum Residual Model</u>, <u>EPA/OPPT Multiple Process Vessel Residual Model</u>, <u>EPA/OPPT Single Vessel Residual Model</u>, <u>EPA/OPPT Small Container Residual Model</u>, <u>EPA/OPPT Solid Residuals in Transport Containers Model</u>, <u>EPA/OPPT Water Saturation Loss Model</u>, User-Defined Loss Rate Model.

Ls [number of manufacturing/ processing/ use lines per site (lines/site)] - input or output for batch operations in the Mass Balance Parameters subtab; input in combination with other batch parameters as option(s) for Amt for cleaning-related release models using loss fractions (LF) and for exposure models using amount handled (AH). <u>EPA/OPPT Bulk Transport Residual Model</u>, <u>EPA/OPPT</u> <u>Drum Residual Model</u>, <u>EPA/OPPT Multiple Process Vessel Residual Model</u>, <u>EPA/OPPT Single Vessel</u> <u>Residual Model</u>, <u>EPA/OPPT Small Container Residual Model</u>, <u>EPA/OPPT Solid Residuals in Transport</u> <u>Containers Model</u>, <u>EPA/OPPT Water Saturation Loss Model</u>, User-Defined Loss Rate Model; <u>EPA/OPPT</u> <u>Small Volume Solids Handling Inhalation Model</u>

m [meters] - unit of measure of length

m2 [square meters] - unit of measure of surface area

m3 [cubic meters] - unit of measure of volume

MCi [mass of material in container handled in a particular activity (kg/container)] - input or output in the Container Parameter subtab; input in combination with other container parameters as option(s) for Amt for container-related release models using loss fractions (LF) and for exposure models

using amount handled (AH). <u>EPA/OPPT Bulk Transport Residual Model</u>, <u>EPA/OPPT Drum Residual Model</u>, <u>EPA/OPPT Small Container Residual Model</u>, <u>EEPA/OPPT Solid Residuals in Transport Containers Model</u>, User-Defined Loss Rate Model; <u>EPA/OPPT Small Volume Solids Handling Inhalation Model</u>

**McE [spray mist capture efficiency (dimensionless)]** - portion of the sprayed mist that is captured out of the air by the spray booth technology; used in the <u>EPA/OPPT Automobile OEM Coating</u> <u>Overspray Loss Model</u>

mg [milligrams] - unit of measure of mass

mi [miles] - unit of measure of length

min [minutes] - unit of measure of time

**MW** [molecular weight of the chemical (g/mol)] - input for the *Chemical* tab; input to all release models that estimate vapor generation using derived mathematical models; input to all inhalation exposure models that use the parameter Cv (MW is used to convert to Cm). <u>EPA/OAQPS AP-42 Loading</u> <u>Model</u>, <u>EPA/OPPT Mass Transfer Coefficient Model</u>, <u>EPA/OPPT Penetration Model</u>; <u>EPA/OPPT Mass</u> <u>Balance Inhalation Model</u>, <u>OSHA PEL-Limiting Model for Substance-Specific Vapors</u>, <u>User-Defined</u> <u>Inhalation Model</u>

MWpel [molecular weight of the chemical with an OSHA PEL that is in the mixture with the assessed chemical (g/mol)] - input for one OSHA PEL substance-specific vapor inhalation exposure model. <u>OSHA PEL-Limiting Model for Substance-Specific Vapors</u>

Nbath [number of bath tanks per site (baths/site)]. <u>Electroplating Bath Additive Use</u> operation.

Nbd [number of batches per site per day (btc/site-day)] - input or output for batch operations in the Mass Balance Parameters subtab; input in combination with other batch parameters as option(s) for Amt for cleaning-related release models using loss fractions (LF) and for exposure models using amount handled (AH). EPA/OPPT Bulk Transport Residual Model, EPA/OPPT Drum Residual Model, EPA/OPPT Multiple Process Vessel Residual Model, EPA/OPPT Single Vessel Residual Model, EPA/OPPT Small Container Residual Model, EPA/OPPT Solid Residuals in Transport Containers Model, EPA/OPPT Water Saturation Loss Model, User-Defined Loss Rate Model; EPA/OPPT Small Volume Solids Handling Inhalation Model

**Nbld [number of batches per line per day (btc/line-day)]** - input or output for batch operations in the *Mass Balance Parameters* subtab

Ncar [number of cars painted per day (cars/site-day)] - input parameter for the <u>Automobile</u> <u>OEM Spray Coating Application</u> operation in the Mass Balance Parameters subtab to determine DMUpaint value

Ncd [number of containers per site per day (containers/site-day)] - input or output in the Container Parameter subtab; input in combination with other batch parameters as option(s) for Amt for container-related release models using loss fractions (LF) and for exposure models using amount handled (AH). <u>EPA/OPPT Bulk Transport Residual Model</u>, <u>EPA/OPPT Drum Residual Model</u>, <u>EPA/OPPT Multiple Process Vessel Residual Model</u>, <u>EPA/OPPT Single Vessel Residual Model</u>, <u>EPA/OPPT Small</u> <u>Container Residual Model</u>, <u>EPA/OPPT Solid Residuals in Transport Containers Model</u>, <u>EPA/OPPT Water</u> <u>Saturation Loss Model</u>, User-Defined Loss Rate Model; <u>EPA/OPPT Small Volume Solids Handling</u> <u>Inhalation Model</u> **Nby [number of batches per site per year (btc/site-yr)]** - input or output for batch operations in the *Mass Balance Parameters* subtab; input as option for Freq for most release models and as option for ED for most exposure models

Ncy [number of containers per year (containers/site-yr)] - input or output for the <u>Operation</u> <u>Parameters Tab -> Container Parameters Subtab</u> as an option for frequency of release (Freq) for release models, as well as for exposure days (ED) for exposure models

**NS** [number of sites (sites)] - input or output for all operations in the *Mass Balance Parameters* subtab; input and output from all release models

**NWexp [number of exposed workers for the source/ activity per site]** - defaults to 3 for most models, and the same value applies to each exposure model for a given source/ activity (e.g., changing the value of NWexp in the dermal model changes the NWexp in the inhalation model to the same value); the appropriate values of 17 for the Auto OEM Spray Coating Inhalation model and 3 for the Auto Refinish Spray Coating Inhalation model have not been incorporated into ChemSTEER; the logic and appropriate default values for this parameter will be finalized in the next version of ChemSTEER

**OD** [operating days per site per year (days/site-yr)] - input or output for all operations in the *Mass Balance Parameters* subtab; input as option for Freq for all release models and as option for ED for all exposure models

**ODa [operating days per site per year for a particular activity (days/site-yr)]** - input or output in the *Container Parameter* subtab; input as option for Freq for all container-related release models and as option for ED for all container-related exposure models

**ODmax [maximum number of operating days possible for batch operations (days/site-yr)]** - input used as a limitation in calculating OD for batch operations in the *Mass Balance Parameters* subtab

**OHa** [operating hours per site per day for a particular activity (hrs/site-day)] - input or output in the *Container Parameter* subtab; input as option for OHa for many release models and as option for h for many exposure models

**P** [total ambient air pressure (torr)] - input to one vapor generation release model. <u>PA/OPPT</u> <u>Penetration Model</u>.

ppm [parts per million] - unit of measure for concentration

**PV** [total production volume of the assessed chemical (kg/yr)] - the overall "volume" of the assessed chemical (in units of mass per time, kg/yr) assessed using ChemSTEER; PV = PVd + PVi (see <u>Chemical Properties Tab</u>.

**PVd [volume of the chemical manufactured domestically (kg/yr)]** - PV = PVd + PVi (see <u>Chemical Properties Tab</u>)

PVf [PERCENT of the total production volume (PV) associated with a particular operation (dimensionless)] - see description of *Percent of PV*, above

PVi [imported volume of the chemical (kg/yr)] - PV = PVd + PVi (see Chemical Properties Tab)

PVop [production volume associated with a particular operation (kg/yr)] (see <u>Operations Tab</u>  $\rightarrow$  Relationships Subtab)

Q [ventilation rate (ft3/min)] - used by the EPA/OPPT Mass Balance Inhalation Model

Qu [quantity of chemical remaining on skin (mg/cm2-event)] - input to all dermal exposure models

r [rate of loading/unloading of containers (containers loaded/hour) or (gallons unloaded/min)] - input or output in the *Container Parameter* subtab; input to one vapor generation release model. <u>EPA/OAQPS AP-42 Loading Model</u>

**R [universal gas constant (82.05 atm cm3/gmol K)]** - input to one vapor generation release model. <u>EPA/OAQPS AP-42 Loading Model</u>

**RinseE [rinsewater recovery efficiency (dimensionless)]** <u>Electroplating Bath Additive Use</u> operation.

**S** [surface area (cm2)] - input to release models that estimate vapor generation from open liquid pools, <u>EPA/OPPT Mass Transfer Coefficient Model</u>, <u>EPA/OPPT Penetration Model</u>

**Sd** [number of shifts worked by each worker per day (shifts/worker-day)] - used to scale the inhalation exposure of workers handling small volumes of solids; <u>EPA/OPPT Small Volume Solids</u> <u>Handling Inhalation Model</u>

sec [seconds] - unit of measure of time

**SrE [solids removal efficiency (dimensionless)]** - fraction of the total solids removed from captured oversprayed paint mist; defaults dependent upon the spray booth technology (i.e., waterwash or dry filter); used by the <u>EPA/OPPT Automobile OEM Coating Overspray Loss Model</u>

**T** [temperature (K)] - input to all release models that estimate vapor generation using derived mathematical models. <u>EPA/OAQPS AP-42 Loading Model</u>, <u>EPA/OPPT Mass Transfer Coefficient Model</u>, <u>EPA/OPPT Penetration Model</u>

**TE [spray gun transfer efficiency (dimensionless)]** - portion of the sprayed coating that adheres to the target surface; dependent upon the type of spray gun (i.e., conventional or HVLP); <u>EPA/OPPT</u> <u>Automobile OEM Coating Overspray Loss Model</u>

**TWA [time-weighted average]** - an average value over the particular time period, usually referring to exposure duration (h) in exposure models

Vbath [volume of solution per electroplating bath (gallons/bath)]. <u>Electroplating Bath Additive</u> <u>Use</u> operation.

**Vc** [volume of the container (gal)] - input or output in the *Container Parameter* subtab; input to release models that estimate vapor generation from vapor displacement, such as filling containers with liquids. <u>EPA/OAQPS AP-42 Loading Model</u>

Vcar [volume of paint used per car (liters/car)] - input for the <u>Automobile OEM Spray Coating</u> <u>Application</u> operation in the Mass Balance Parameters subtab; used with Dprod and Ncar to calculate DMUpaint

**Vm [molar volume of gas (L/mol)]** - input to all inhalation exposure models that use the parameter Cv (Vm used to convert to Cm); default value of 24.45 assumes ambient conditions of 25°C and 1 atm. <u>EPA/OPPT Mass Balance Inhalation Model</u>; <u>OSHA PEL-Limiting Model for Substance-Specific Vapors</u>, <u>User-Defined Inhalation Model</u>

**Vpaint [volume of paint used per day (gallons/site-day)]** - input for the <u>Automobile OEM Spray</u> <u>Coating Application</u> operation in the *Mass Balance Parameters* subtab; used with Dprod and a conversion of gallons to liters to calculate DMUpaint

**VPchem [vapor pressure of the pure chemical (torr)]** - input for the *Chemical* tab; input to all release models that estimate vapor generation using derived mathematical models; input to equation

for calculating the maximum possible volumetric vapor concentration for two inhalation exposure models. <u>EPA/OAQPS AP-42 Loading Model</u>, <u>EPA/OPPT Mass Transfer Coefficient Model</u>, <u>EPA/OPPT</u> <u>Penetration Model</u>; <u>EPA/OPPT Mass Balance Inhalation Model</u>, <u>OSHA PEL-Limiting Model for Substance-Specific Vapors</u>

VPpel [vapor pressure of the chemical with an OSHA PEL that is in the mixture with the assessed chemical (torr)] - input for the OSHA PEL-Limiting Model for Substance-Specific Vapors

vz [air speed (ft/min)] - input to release models that estimate vapor generation from open liquid pools; input to equation for calculating ventilation rate default for one inhalation exposure model. EPA/OPPT Mass Transfer Coefficient Model, EPA/OPPT Penetration Model, EPA/OPPT Mass Balance Inhalation Model

WSchem [water solubility of the pure chemical (g/L)] - input for the *Chemical* tab; input to one release model. <u>EPA/OPPT Water Saturation Loss Model</u>

**X** [vapor pressure correction factor (dimensionless)] - input to all release models that estimate vapor generation using derived mathematical models and having the VP parameter; input to equation for calculating the maximum possible volumetric vapor concentration for two inhalation exposure models. . <u>EPA/OAQPS AP-42 Loading Model</u>, <u>EPA/OPPT Mass Transfer Coefficient Model</u>, <u>EPA/OPPT Penetration Model</u>, <u>EPA/OPPT Mass Balance Inhalation Model</u>; <u>OSHA PEL-Limiting Model for Substance-Specific Vapors</u>.

Xother [vapor pressure correction factor for process material that is neither raw material, nor product (dimensionless)] - input (as a possible non-default value for X) to vapor generation release models using derived mathematical models and having the VP parameter; input to calculation for calculating the maximum possible volumetric vapor concentration for two inhalation exposure models. EPA/OAQPS AP-42 Loading Model, EPA/OPPT Mass Transfer Coefficient Model, EPA/OPPT Penetration Model; EPA/OPPT Mass Balance Inhalation Model, OSHA PEL-Limiting Model for Substance-Specific Vapors. Default options for calculating Xother are contained in the Operation Parameters Tab → Shared Parameters/Factors Subtab.

**Xprod [vapor pressure correction factor for the product material (dimensionless)]** - input (as a possible default value for X) to vapor generation release models using derived mathematical models and having the VP parameter; input to calculation for calculating the maximum possible volumetric vapor concentration for two inhalation exposure models. <u>EPA/OAQPS AP-42 Loading Model, EPA/OPPT Mass</u> <u>Transfer Coefficient Model, EPA/OPPT Penetration Model; EPA/OPPT Mass Balance Inhalation Model, OSHA PEL-Limiting Model for Substance-Specific Vapors</u>. Default options and calculating for Xprod are contained in the <u>Operation Parameters Tab</u> → Shared Parameters/Factors Subtab.

Xrm [vapor pressure correction factor for the raw material (dimensionless)] - input (as a possible default value for X) to vapor generation release models using derived mathematical models and having the VP parameter; input to calculation for calculating the maximum possible volumetric vapor concentration for two inhalation exposure models. EPA/OAQPS AP-42 Loading Model, EPA/OPPT Mass Transfer Coefficient Model, EPA/OPPT Penetration Model; EPA/OPPT Mass Balance Inhalation Model, OSHA PEL-Limiting Model for Substance-Specific Vapors. Default options and calculating for Xprod are contained in the Operation Parameters Tab → Shared Parameters/Factors Subtab.

Yaddtv [weight fraction of the chemical in the electroplating batch additive (dimensionless)]. <u>Electroplating Bath Additive Use</u>.

Ybath [weight fraction of the chemical in the electroplating bath (dimensionless)]. <u>Electroplating Bath Additive Use</u>. Yderm [weight fraction of the chemical in liquid or solid (dimensionless)] - input to all dermal exposure models

**Yfpaint [weight fraction of the chemical in the formulated paint (dimensionless)]** - input parameter for the <u>Automobile Refinish Spray Coating Application</u> operation; only used in cases where the user elects an effluent basis for the operation Mass Balance Parameter calculations (this is the nondefault option for this operation); used by inhalation and dermal exposure models

Yi [weight fraction of the chemical in material handled in a particular activity (dimensionless)] - input or output in the *Container Parameter* subtab; input in combination with other container parameters as option(s) for Amt for container-related release models using loss fractions (LF); input for inhalation exposure models using amount handled (AH) or OSHA PELs for container-related sources/ activities, and for all dermal models for container-related sources/ activities. <u>EPA/OPPT Bulk Transport</u> <u>Residual Model</u>, <u>EPA/OPPT Drum Residual Model</u>, <u>EPA/OPPT Small Container Residual Model</u>, <u>EPA/OPPT Solid Residuals in Transport Containers Model</u>, User-Defined Loss Rate Model; <u>EPA/OPPT Small Volume</u> <u>Solids Handling Inhalation Model</u>, <u>OSHA PEL-Limiting Model for Substance-Specific Particulates</u>, <u>OSHA</u> <u>PEL-Limiting Model for Substance-Specific Vapors</u>, <u>OSHA Total PNOR PEL-Limiting Model</u>, <u>OSHA</u> <u>Respirable PNOR PEL-Limiting Model</u>

Yliq [weight fraction of the chemical in liquid (dimensionless)] - input to all dermal exposure models

**Ypaint [weight fraction of the chemical in the paint (dimensionless)]** - input and output for the <u>Automobile OEM Spray Coating Application</u> operation in the *Mass Balance Parameters* subtab; used by the inhalation and dermal exposure models

**Ypel [weight fraction of the chemical with an OSHA PEL that is in the particulate or mixture with the assessed chemical (dimensionless)]** - input for all OSHA PEL substance-specific inhalation exposure models. <u>OSHA PEL-Limiting Model for Substance-Specific Particulates</u>, <u>OSHA PEL-Limiting Model for Substance-Specific Vapors</u>

**Yppaint [weight fraction of the chemical in the purchased paint (dimensionless)]** - input and output for the <u>Automobile Refinish Spray Coating Application</u> operation in the *Mass Balance Parameters* subtab; used by the inhalation and dermal exposure models

**Yprod [weight fraction of the chemical in the product (dimensionless)]** - input or output for all operations in the *Mass Balance Parameters* subtab; input as default for Yi for product related container sources/ activities in the *Container Parameter* subtab; input as option for Ys and Yderm for most exposure models

yr [years] - unit of time

Yrinse [weight fraction of the chemical in the electroplating batch rinse water (dimensionless)]. <u>Electroplating Bath Additive Use</u> operation.

**Yrm [weight fraction of the chemical in the raw material (dimensionless)]** - input or output for all operations in the *Mass Balance Parameters* subtab; input as default for Yi for product related container sources/ activities in the *Container Parameter* subtab; input as option for Ys and Yderm for most exposure models

**Ys [weight fraction of the chemical in particulate or mixture (dimensionless)]** - input for all particulate and OSHA PEL inhalation exposure models. <u>EPA/OPPT Small Volume Solids Handling</u> Inhalation Model, EPA/OPPT Mass Balance Inhalation Model, OSHA PEL-Limiting Model for Substance<u>Specific Particulates</u>, <u>OSHA PEL-Limiting Model for Substance-Specific Vapors</u>, <u>OSHA Total PNOR PEL-</u> <u>Limiting Model</u>, <u>OSHA Respirable PNOR PEL-Limiting Model</u>

**Ysf [weight fraction of the solids within the paint (dimensionless)]** - used in the <u>EPA/OPPT</u> <u>Automobile Spray Coating Inhalation Exposure Model</u>

# **CHEMSTEER TERMS**

The following list includes many of the key terms used in ChemSTEER and is in alphabetical order. In future ChemSTEER User Guides, you will be able to click on the link of interest following a term's description to access information about the term and how it is used in ChemSTEER.

Activity - see Release Source/ Exposure Activity definition below.

Chemical - the chemical being assessed.

Dermal - skin

**Exposure** - contact of the assessed chemical with a boundary of a human. In ChemSTEER, the human is a worker, and the boundaries are the respiratory and upper digestive tracts for inhalation exposure and the skin, usually one or both hands, for dermal exposure.

**Exposure Activity** - see *Release Source/ Exposure Activity* definition below.

**Percent of PV** - PERCENT of the assessed volume (PV) that flows to or from the operation. For example, if a manufacturing operation (User-defined Manufacturing) produces all of the assessed volume, then the Percent of PV for User-defined Manufacturing is 100 (100%). If there are two primary use operations (User-defined Use and User-defined Use 2) that use the chemical, and three quarters is used by the first use operation and the remainder by the second use operation, then the Percent of PV for User-defined Use is 75 (75%) and the Percent of PV for User-defined Use 2 is 25 (25%). (see Operations Tab  $\rightarrow$  Relationships Subtab)

**Input (to a model or to another equation in ChemSTEER)** - a parameter or value of a parameter used in a release or exposure model equation or to an equation used in ChemSTEER to calculate a result (output) from one or more equations calculating release or exposure related parameter values.

**Manufacturing** - generally represents an operation in which the chemical being assessed is created or formed in a reaction.

Method - synonymous with Model

**Model** - an equation or set of equations containing parameters related to chemical- and operation-specific factors, and the equation(s) are used to calculate estimated amounts (quantities) of release of and worker exposure to the assessed chemical.

**Operation** - a workplace or set of "homogeneous" workplaces with essentially the same (or similar) processes, equipment, chemical throughputs, procedures, and worker populations, such that estimates of releases and exposures to the chemical being assessed can be assumed to be essentially the same for all of the workplaces, if more than one, in the set. If workplaces differ in some aspects that could result in significantly different estimates of releases and exposures, you should assess these workplaces as two or more separate operations.

**Output (from a model or from another equation in ChemSTEER)** - a parameter or value (result) of a parameter calculated using one or more equations in a release or exposure model or from an equation used in ChemSTEER to generate release or exposure related parameter values.

**Processing** - generally represents an operation in which the chemical being assessed is not created or formed and in which the chemical being assessed is not destroyed or transformed in a chemical reaction, or otherwise becomes essentially unavailable for further release or exposure. Formulation and repackaging operations would usually be considered to be types of Processing operations.

**Product** - material leaving the operation, whether pure chemical or chemical in a mixture. The product from an operation is assumed to be the raw material of any subsequent operation(s).

**Production Volume** - the overall "volume" of the assessed chemical (in units of mass per time, kg/yr) assessed using ChemSTEER; PV = PVd + Pvi. (see <u>Chemical Properties Tab</u>)

**Raw Material** - material entering the operation, whether pure chemical or chemical in a mixture. The product from an operation is assumed to be the raw material of any subsequent operation(s).

**Relationship** - how different workplaces are related as suppliers and customers. A customer's operation receiving the chemical being assessed, whether pure or in a mixture with other chemicals, from a supplier makes the customer's operation a subsequent operation to the supplier's operation.

**Release (environmental release)** - chemical emission or disposal to the environment or to treatment or disposal facilities outside of the operation.

**Release Source/ Exposure Activity** - sources and activities in an operation that can/ do/ will cause releases to the environment and/ or worker exposures. Most Source/ Activities have one or more default models that ChemSTEER uses to estimate releases and exposures. Choosing appropriate Source/ Activities allow you to access models to make these estimates.

**Result** - see *Output* definition above.

TWA - time-weighted average, usually referring to exposure duration (h).

**Use** - generally represents an operation in which the chemical being assessed destroyed or transformed in a chemical reaction, or otherwise becomes essentially unavailable for further release or exposure.

# References

The methods and models used in ChemSTEER are from several EPA sources, including the "Chemical Engineering Branch Manual for the Preparation of Engineering Assessments" and other reports and memoranda detailing the methods used in CEB assessments. References to the industryspecific operations are taken from the "Chemical Engineering Branch Compilation of Generic Scenarios for Chemical Uses." These references document the various empirical, mathematical, and suppositional methods and models that have been developed and used by EPA over many years of workplace exposure and release assessment.

Click on the following links to access the files containing copies of the relevant portions of these references.

NOTE: These files are in Adobe's Portable Document Format (PDF). To view or print them you will need to have the Adobe Acrobat Reader program installed on your computer. The Reader can be downloaded and used with no charge; for more information at EPA about PDF files, click the following link: http://www.epa.gov/epahome/pdf.html

US EPA Memo entitled <u>Updating CEB's Method for Screening-Level Assessments of Dermal Exposure</u>, September 2013.

Pre-publication draft article entitled <u>Evaporation of Pure Liquids From Open Surfaces</u>, Fredric C. Arnold and Alfred J. Engel, US EPA, October, 1999.

SAIC for US EPA/OPPT. Generic Scenario for Automobile Spray Coating Draft Report. August 1996.

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Fehrenbacher, M.C. and Hummel, A.A. "Evaluation of the Mass Balance Model Used by the Environmental Protection Agency for Estimating Inhalation Exposure to New Chemical Substances". American Industrial Hygiene Association Journal. June 1996. 57: 526-536.

Organization for Economic Co-operation and Development. <u>Emission Scenario Document on Coating</u> <u>Application via Spray Painting in the Automotive Refinishing Industry</u>. June 2010.

US EPA Memo entitled <u>Draft Guidance on LADDs and APDRs</u>, from Becky Brown, Chemical Engineering Branch, to Chemical Engineering Branch Staff and Management. 6/21/93.

US EPA Chemical Engineering Branch Generic Scenario entitled <u>Textile Dyeing</u>, 10/15/92.

US EPA Memo entitled <u>Standard Assumptions for PMN Assessments</u>, from the Chemical Engineering Branch Quality Panel to Chemical Engineering Branch Staff and Management. 10/92.

<u>Chapter 4 of Chemical Engineering Branch Manual for the Preparation of Engineering Assessments</u>, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991. <u>Chapter 7 of the Chemical Engineering Branch Manual for the Preparation of Engineering Assessments;</u> Washington, DC; Office of Toxic Substances, U.S. Environmental Protection Agency; 1991; pp. 7-3 through 7-9.

Appendix K of Chemical Engineering Branch Manual for the Preparation of Engineering Assessments, Washington, D.C.: Office of Toxic Substances, U.S. Environmental Protection Agency, 1991.

PEI Associates for US EPA/OTS. <u>Releases During Cleaning of Equipment</u>. July 1988.

Generic Scenario: Roll Coating of UV-Curable Coatings. No date.

Summary Sheet: Recirculating Water-Cooling Tower, No date.

US EPA Chemical Engineering Branch model entitled, <u>Generic Model to Estimate Dust Releases from</u> <u>Transfer/Unloading Operations of Solid Powders</u>; July 20, 2007.

# Appendix A - Industry Specific Operations

The following sections provide details on the hardcoded industry-specific Generic Scenarios included in ChemSTEER.

# **AUTOMOBILE ORIGINAL EQUIPMENT MANUFACTURE (OEM) SPRAY COATING**

Revised August 12, 2003. This operation is applicable to the use of a liquid coating product (e.g., paint) that is sprayed onto originally manufactured (i.e., new) automobile surfaces. It estimates the releases and exposures to <u>nonvolatile</u> components of the coating only. The draft *Generic Scenario for Automobile Spray Painting*, August 1996, was the primary reference source for the operation defaults described below.

By default, this operation will assume the use of a <u>conventional spray gun</u> within a <u>downdraft</u> <u>spray booth</u> having a <u>waterwash curtain</u>. These specifications determine default input parameter values used by the release and exposure models. You may specify the *spray gun type* for the operation in the <u>Operation Parameters Tab</u>  $\rightarrow$  <u>Shared Parameters/Factors Subtab</u>. Non-default values for model parameters affected by the *booth ventilation type* and/or the *overspray control device* may be specified at the *Release* or *Exposure* tab.

## Operation tab / Description subtab

## Selected NAICS (default)

The following NAICS codes are pre-selected for this operation:

- 3361 Motor Vehicle Manufacturing
- 3362 Motor Vehicle Body and Trailer Manufacturing

## **Process Description**

NOTE: Release sources and exposure activities prior to the spray coating step of this operation (e.g., unloading of containers, equipment cleaning) are not included and must be manually selected. Pre-coating steps have not been researched, and those steps in the following description are presumed.

This operation assumes that the coating product is primarily applied via robotic devices and that worker exposures during the coating step are the result of manual touch-up of parts damaged during assembly.

The coating product is shipped to automotive OEM facilities in bulk containers (tank trucks, totes, drums, etc.) Depending on the facility, the coating may be unloaded into a storage tank until use or stored in the original container. Prior to the application, the coating may be further blended in a mixing tank with other additives and solvent to achieve optimum viscosity and color.

The formulated coating is than loaded to a feed tank connected to robotic controlled spray guns and is spray applied onto cars. Painted cars are cured in a room where the temperature can reach 450F. Several layers of coating are applied to car alternated with heating to cure the coating or drive off moisture. After the curing, no further exposure to or release of the coating are expected.

Although the automobile OEM spray coating process is highly automated, some "touch-ups" are expected including the repair of scratches and damages that may result during the assembly activities. These repairs are usually performed by workers using spray guns in downdraft booths.

Worker exposure to paint may occur during transfer of coatings from shipping containers to a storage tank, blending of coating, manual spray application, and clean-up. Sources for potential environmental releases include stack air release during the spray application, solid and aqueous waste of oversprayed mist, clean-up waste and empty containers.

The default process description for this operation is as follows:

Unload coating product containing the assessed chemical from shipping container -> Mix and/or store (optional) -> Transfer to spray gun feed system -> Apply coating to automobile surfaces (some sprayed coating does not remain on the surfaces - it passes into the booth ventilation system and is either captured in exhaust controls or is exhausted into the air through the stack) -> Bake/cure coating at high temperatures (assessed chemical is destroyed or fixed to the coated surface).

## Operation tab / Sources/Activities subtab

The following default source/activity is automatically listed on the *Sources/Activities* that will be assessed in the operation list on the *Update Operation Sources/Activities* screen (launched by the *Update Sources/Activities* button):

<u>Automobile OEM Spray Coating Application</u> (Exposure - Yes, Release - Yes)

## **Available Activities:**

• All other activities

# Operation Parameters tab / Mass Balance subtab

Clicking the *Update Parameters* button on the *Mass Balance Parameters* subtab launches the *Update Operation Mass Balance Parameter* screen. The following logic defines the default conditions and parameter values for this screen.

## Mass Balance Basis Selection tab

Default selections are *Continuous* and *Formulated Paint Usage* (where Formulated Paint Usage replaces Product since the basis is actually the paint used rather than a true product).

## **Specify Mass Balance Input Parameters**

If you select a different basis other than the default basis selection (*Continuous and Formulated Paint Usage*), ChemSTEER uses the logic and calculations associated with user-defined operations, which are described in the <u>Operation Parameters Tab</u>  $\rightarrow$  <u>Mass Balance Parameters Subtab</u> pages of the User Guide. You must manually make all mass balance calculations by substituting the parameters for formulated paint used in place of standard product output parameters from that logic, and the logic and default calculations below for this operation are not used.

If you retain the default basis selection (*Continuous and Formulated Paint Usage*), the parameters listed below and the following logic are used to perform mass balance calculations.

## Parameters

NOTE: The equivalent parameter in the Generic Scenario for Automobile Spray Coating, if applicable, appears in parentheses.

	DMIrm:	Daily mass input of raw material (kg/site-day)
	DMIchem:	Daily mass input of the chemical (kg/site-day)
	DMUfpaint:	Daily mass of formulated coating used (DMUfpaint replaces DMOprod for user- defined operations, but for the purpose of the mass balance is used in the same way) (kg/site-day) (0 < DMUpaint)
	DMUchem:	Daily mass of chemical in the formulated coating used (DMUchem replaces DMOchem for user-defined operations, but for the purpose of the mass balance is used in the same way) (kg/site-day) (0 < DMUchem)
	Yrm:	Weight fraction of the chemical in raw material (0 < Yrm < 1; default: Yprod from previous operation)
	Yfpaint (C):	Weight fraction of the chemical in the formulated paint (Yfpaint replaces Yprod for user-defined operations, but for the purpose of the mass balance is used in the same way) (0 < Ypaint < 1; default: Yrm)
	NS (Nsites):	Number of sites (integer > 0)
OD	: Drm:	Number of operating days (days/site-yr) (integer, 0 < OD < 365; default: 250) Density of raw material (default; Dprod from the previous operation container parameter or mass balance, or, if no previous value available, 1) (kg/liter)
	Dfpaint:	Density of formulated paint (Dfpaint replaces Dprod for user-defined operations, but for the purpose of the mass balance is used in the same way) (kg/liter) (default: Drm)
	Vcar:	Volume of coating used per car (Liters/car) (Vcar > 0; default: 8 L/car)
	Ncar:	Number of cars spray coated per site-day (Ncar > 0; default: 664 cars/site-day based on 166,000 cars/site-yr and 250 days/site-yr)
	DVUfpaint:	Volume of formulated coating used per day (gallons/site-day) (DVUfpaint > 0)

These parameters are used to perform mass balance calculations on the ChemSTEER Operation Parameters windows as described by the default value calculations for this industry operation listed below. If you choose to update any default values, ChemSTEER updates other values using the logic and calculations described in the <u>Operation Parameters Tab  $\rightarrow$  Mass Balance Parameters Subtab</u> pages of the User Guide (where the formulated paint parameters in the list above replace standard product output parameters from that logic). Clicking the Restore defaults button will turn off the fix boxes set for any of the parameters, clear the values for all parameters on this screen, and replace them with the default values based on the logic and calculations listed below.

## **Default Calculations**

Default values for the mass balance parameters for this industry operation are calculated based upon the following logic and calculations.

- 1. Yfpaint = Yrm = Yprod from previous operation.
- 2. DMUfpaint = Vcar x Dfpaint x Ncar (using default values shown in parameter list above).
- 3. DMUchem = DMUfpaint x Yfpaint.
- 4. If PVop < DMUchem x OD, then NS = 1

If PVop > DMUchem x OD, then NS = PVop / (DMUchem x OD) ; If NS is not calculated to be an exact integer, it will be rounded up to the next highest integer above PVop / (DMUchem x OD).

- 5. OD = PVop / NS / DMUchem
- 6. DMIchem = DMUchem
- 7. DMIrm = DMIchem / Yrm

A primary calculation for this operation is DMUfpaint (daily mass of formulated coating used). You may revise DMUfpaint by checking the fix box for DMUpaint, which activates the Calculate button next to the display box for the value of this parameter. Clicking on this *Calculate* button launches the *Update Mass of Formulated Paint Used* window.

In this window you have the option of choosing between two methods of calculating DMUfpaint. You have the option of retaining or updating the values of any of the parameters used by the method that is selected. The first method uses the equation:

DMUfpaint = Vcar (liters of paint/car) x Dfprod (formulated coating density, kg/L) x Ncar (number of cars/site-day).

The second method uses the equation:

DMUfpaint = VMUfpaint (gallons of formulated coating/site-day) x Dfpaint (formulated coating density, kg/L) x 3.785 L/gal.

Clicking the *Restore defaults* button will clear the values for all parameters on this screen and replace them with the default values based on the information and logic listed above.

You may retain or update the values of any of the parameters used by the method that is selected.

# Operation Parameters tab / Shared Parameters/Factors subtab

When the Automobile OEM Spray Coating operation is selected, the Shared Parameters/Factors subtab will display the Automotive Spray Coating shared parameter/factor, Spray Gun Type, by default. The user may change the Spray Gun Type default value by double-clicking on it in the table. The Automobile OEM Spray Coating default setting, as well as the non-default option is summarized for the shared Spray Gun Type in the table below:

Shared Parameter/Factor	Default Value/Setting	Non-default Option
Spray Gun Type	Conventional*	HVLP

\*The conventional spray gun default for the Automobile OEM Spray Coating Operation was adopted as an internal policy decision in July 2003.

## **Releases Tab**

For the *Automotive OEM Spray Coating Application* source/activity, the default multi-media release model is the <u>EPA/OPPT Automobile OEM Coating Overspray Loss Model</u>.

## Exposures Tab

For the Automotive OEM Spray Coating Application source/ activity:

• The overriding default for this worker activity: NWexp = 17 workers per site.

The default dermal exposure model is the <u>US EPA Memo entitled Updating CEB's Method for</u> <u>Screening-Level Assessments of Dermal Exposure, September 2013.</u>

- EPA/OPPT 2-Hand Dermal Immersion with Liquid Model.
- The default inhalation exposure model is the <u>EPA/OPPT Automobile OEM Spray Coating</u> <u>Inhalation Exposure Model</u>.

## References

SAIC for US EPA/OPPT. <u>Generic Scenario for Automobile Spray Coating Draft Report</u>. August 1996.

# **ELECTROPLATING BATH ADDITIVE USE**

Revised April 14, 2004. This operation is applicable to the use of a material that is added to an electroplating bath. *Electroplating* is the process by which a metal coating is applied to an object immersed in an electrolytic solution (i.e., the bath) by passing a current through the solution (the article to be plated is the cathode). This operation also applies to *anodizing* (wherein the surface to be plated is the anode) and *electroless* or *autocatalytic plating* (wherein a chemical reducing agent is used to reduce a dissolved metal onto a surface without the use of an electric current). This operation estimates the releases of and worker exposure to a chemical contained in the bath additive. The August 1996 *Generic Scenario: Electroplating* document was the primary reference source for the operation defaults described below.

## Operations tab $\rightarrow$ Description subtab

## Selected NAICS

The following NAICS code is pre-selected for this operation:

• 332813 – Electroplating, Plating, Polishing, Anodizing, and Coloring

## **Process Description**

NOTE: Release sources and exposure activities prior to the charging step of this operation (e.g., unloading of containers, empty container cleaning/disposal) are not included and must be manually selected.

The process begins with several pre-treatment cleaning steps including immersion and spray rinses of the parts to be plated. These pretreatment steps typically utilize deionized water and alkaline or acidic solutions. The parts are then dipped into the plating bath, which consists of the metal ions in solution (as provided by dissolved metal from the anode or metal salts/oxides), complexing agents, stabilizers to prevent hydrolysis, buffers for pH maintenance, and catalysts.

These additive chemical concentrations range from amounts measured in ppm for brighteners up to 20 percent for metal salts. Electroplating baths are almost always aqueous-based.

The dip time and bath size depend on the metal to be plated, the thickness of the desired coating, and the size and shape of the immersed part. After dipping, the part is then rinsed by several more immersion and spray rinses with deionized and permeate water. The part is then baked to cure the coating.

Although electroplating includes all of the stages mentioned above, this operation applies only to plating followed by rinsing.

The additives are usually nonvolatile and tend to remain in the bath. The baths, however, are equipped with exhaust systems for any vapors that may exist above the solution surface. Worker exposure may occur during transfer of the additive from shipping containers to recharge the dip tanks. The worker may also be exposed to additive materials during sampling or other activities wherein evolved hydrogen and oxygen gas rising from the submerged part, the anode, or the cathode, as well as from the residual bath solution dragged with the part into the air. Sources for potential environmental

releases include discharge of waste rinsing materials and spent baths. There may also be releases from container residues and potentially from the pre-treatment cleaning steps; both must be manually assessed.

The default process description for this operation is as follows:

Pre-treatment cleaning steps (not assessed by this operation) -> Transfer of additive containing the chemical from shipping container into dip tank (you must manually add or adjust unloading and cleaning activities based on the loading activity in the previous operation) -> Electroplate surfaces of parts-> Plated parts immersed in rinse tanks and spray rinsed -> Bake/cure plated coating (chemical is either destroyed or fixed to the coated surface)

## Operations tab / Sources/Activities subtab

The following default sources/activities are automatically listed on the Sources/Activities that will be assessed in the operation list on the Update Operation Sources/Activities screen (launched by the Update Sources/Activities button):

- <u>Changing Electroplating Bath</u> (Exposure No, Release Yes)
- <u>Rinsing Electroplated Parts</u> (Exposure No, Release Yes)
- <u>Operating the Electroplating Bath</u> (Exposure Yes, Release No)

## Available Activities

• All other activities

NOTE: The *Charging Electroplating Batch, Rinsing Electroplated Parts, and Operating the Electroplating Batch* source/activities may not be used for any operation other than the Electroplating Batch Additive Use operation.

## Operation Parameters tab / Mass Balance subtab

Clicking the Update Parameters button on the Mass Balance Parameters subtab launches the Update Operation Mass Balance Parameter screen. The following logic defines the default conditions and parameter values for this screen.

## Mass Balance Basis Selection tab

Default selections are *Continuous* and *Electroplating Bath Additive Usage* (where Electroplating Bath Additive Usage replaces Product since the basis is actually the chemical additive used in the bath solution rather than a true Product).

## **Specify Mass Balance Input Parameters**

If you select a different basis other than the default basis selection (*Continuous* and *Electroplating Bath Additive Usage*), ChemSTEER uses the logic and calculations (with user-defined processing rules) described in the *Entering/Updating Mass Balance Parameters* pages of the User Guide. The user must manually make all mass balance calculations by substituting the parameters for the

amount of additive used in place of standard product output parameters from that logic, and the logic and default calculations below for this operations are not used.

For this scenario, if the default basis selection is retained (*Continuous* and *Electroplating Bath Additive Usage*), the Specify Mass Balance Input Parameters screen will have two non-standard text changes.

1) The "Calculate remaining two parameters" button is re-labeled "Calculate remaining parameters"

2) The standard mass balance instruction text at the top of the screen is changed to "Please specify at least one (maximum three) of the first five parameters. ChemSTEER will calculate the remaining parameters for you."

If you retain the default basis selection, the parameters listed below and the following logic are used to perform mass balance calculations.

Parameters	
DMIrm:	Daily mass input of raw material (kg/site-day)
DMIchem:	Daily mass input of the chemical (kg/site-day)
ADMUaddtv:	Averaged daily mass of the bath additive used to replace intermittent losses from bath changes and daily losses from rinsing parts (ADMUaddtve replaces DMOprod for user-defined operations, but for the purpose of the mass balance is used in the same way) (kg/site-day) (0 < ADMUaddtve) (default based on equations presented below)
ADMUchem:	Averaged daily mass of chemical in the bath additive used to replace intermittent losses from bath changes and daily losses from rinsing parts (ADMUchem replaces DMOchem for user-defined operations, but for the purpose of the mass balance is used in the same way) (kg/site-day) (0 < ADMUchem) (Read-only, default based on equations presented below; ADMUchem can only be updated by modifying changeable parameters on the update ADMUchem screen.)
Yrm:	Weight fraction of the chemical in raw material ( $0 < Yrm \le 1$ ; default: Yprod from previous operation or, if no previous operation, 1)
Yaddtv:	Weight fraction of the chemical in the additive (Yaddtve replaces Yprod for user-defined operations, but for the purpose of the mass balance is used in the same way) ( $0 < Yaddtve \le 1$ ; default: Yrm)
NS:	Number of sites (integer > 0) (default based on equations presented below)
OD:	Number of operating days (days/site-yr) (integer, $0 \le OD \le 365$ ; default: 250)
Ybath:	Weight fraction of the chemical in the bath (0 < Ybath $\leq$ 1; default: 0.0434)
Yrinse:	Weight fraction of the chemical in the rinse water (0 < Yrinse < 1 and < Ybath; default: 0.0235 or Ybath x 0.50, if user-defined Ybath)
Dbath:	Density of the bath (kg/liter) (default: 1)

Drinse:	Density of the rinse (kg/liter) (default: 1)
Vbath:	Volume of solution per bath (gallons/bath) (Vbath < 0; default: 2,500)
Nbath:	Number of bath tanks per site (baths/site) (default: 3)
Freqbath:	Frequency of bath changes per year (changes/bath/yr) (Freqbath $\geq$ 0; default: 2)
DVrinse:	Daily volume of rinse water generated per site (gallons/site-day) (DVrinse > 0; default: 4932)
RinseE:	Rinsewater recovery efficiency (0 < RinseE < 1; default: 0.90)
EPVop:	Estimated PVop for iterative calculation sequences.

These parameters are used to perform mass balance calculations for this industry operation on the ChemSTEER *Operation Parameters* windows using the logic and calculations described below. Clicking the *Calculate* button next to ADMUchem in the *Specify Mass Balance Input Parameters* subtab will allow you to review or modify additional mass balance parameters for this operation by activating the *Update Average Daily Mass of Chemical Used* window. Clicking the *Restore defaults* button in the *Update Average Daily Mass of Chemical Used* window will turn off the fix boxes set for any of the parameters <u>except</u> Yrinse (which remains checked), clear the values for all parameters on this screen, and replace them with the default values shown above and based on the logic and calculations described below.

Default values for the mass balance parameters for this industry operation are calculated based upon the following logic and calculations, where Vbath, Nbath, Freqbath, Dbath, Ybath, OD, DVrinse, Drinse, Yrinse (fix box checked by default on the *Update Average Daily Mass of Chemical Used* window), and RinseE are initially set to the default values given in the parameter list above.

- EP1. ADMUchem = [(Vbath x Nbath x Freqbath x Dbath x 3.78 L/gal x Ybath / OD) + (DVrinse x Drinse x 3.78 L/gal x Yrinse x (1 RinseE))]
- EP2. NS = PVop / OD / ADMUchem

If NS is not calculated to be an exact integer, NS is rounded up to the next highest integer above PVop / OD / ADMUchem. If NS is calculated to be less than 1, it is rounded up to 1 site and OD is recalculated using EP2a (note that EP2a can also be used to resolve mass balance discrepancies in cases where ADMUchem is directly fixed or set by the selection of Yaddtv and ADMUaddtv fix boxes):

- EP2a. OD = PVop / NS / ADMUchem
- EP3. ADMUchem = PVop / NS / OD (resolves discrepancies due to rounding of NS)

Note: The read-only value of ADMUchem is only re-adjusted if it is not fixed (i.e., the read-only of ADMUchem will be set by the fix box; however, non-user specified values of changeable parameters used to calculate ADMUchem can be adjusted based on the sequences described below - with the value of ADMUchem unchanged).

- EP4. Yaddtv = Yrm = Yprod from previous operation (or 1 if no previous operation)
- EP5. ADMUaddtv = ADMUchem / Yaddtv
- EP6. DMIchem = ADMUchem

EP7. DMIrm = DMIchem / Yrm

Because ADMUchem and OD are related both by the primary equation EP1 for electroplating and by the standard mass balance equation EP3, ChemSTEER recalculates parameters in EP1 to maintain the mass balance after each recalculation of ADMUchem from equations other than EP1. These recalculations depend upon fix box conditions and are shown in Sequences A, B, C, and D below. To complete the calculation of default values, ChemSTEER uses Sequence A.

## Mass Balance Maintenance Sequences A, B, C, and D

Sequence A - Both Vbath and DVrinse fix boxes are NOT checked.

ChemSTEER solves for Vbath and DVrinse with the assumption DVrinse = Vbath x Nbath x 4932 / 7500 (ratio of default values in the reference document):

Vbath=ADMUchem / [(Nbath x Freqbath x Dbath x 3.78 x Ybath / OD) +<br/>(4932 / 7500 x Nbath x Drinse x 3.78 x Yrinse x (1-RinseE))]DVrinse=(4932 / 7500) x Nbath x VbathSequence B - Vbath fix box is checked and DVrinse fix box is NOT checked.

ChemSTEER solves for DVrinse:

DVrinse =[ADMUchem - (Vbath x Nbath x Freqbath x Dbath x 3.78 L/gal x Ybath / OD)] / (Drinse x 3.78 L/gal x Yrinse x (1 - RinseE))

If DVrinse < 0, then DVrinse = 0. A pop-up warning window with the message "Parameters should be adjusted such that ADMUchem is increased and/or Vbath is decreased" appears and clicking *OK* removes the window. This message appears both at the bottom of the *Update Average Daily Mass of Chemical Used* window and at the bottom of the *Specify Mass Balance Input Parameters* subtab.

Sequence C - Vbath fix box is NOT checked and DVrinse fix box is checked.

ChemSTEER solves for Vbath:

Vbath =[ADMUchem - (DVrinse x Drinse x 3.78 L/gal x Yrinse x (1 - RinseE))] / (Nbath x Freqbath x Dbath x 3.78 L/gal x Ybath / OD)

If Vbath < 0, then Vbath = 0. A pop-up warning window with the message "Parameters should be adjusted such that ADMUchem is increased and/or DVrinse is decreased" appears and clicking *OK* removes the window. This message appears both at the bottom of the *Update Average Daily Mass of Chemical Used* window and at the bottom of the *Specify Mass Balance Input Parameters* subtab.

Sequence D - Both Vbath and DVrinse fix boxes ARE checked.

ChemSTEER checks for mass balance discrepancies:

If the absolute value of

[ADMUchem - ((Vbath x Nbath x Freqbath x Dbath x 3.78 L/gal x Ybath / OD) + (DVrinse x Drinse x 3.78 L/gal x Yrinse x (1 - RinseE))) / ADMUchem]

is greater than 0.05, a pop-up warning window with the message "The fixed values of DVrinse and Vbath result in a mass balance discrepancy of greater than 5%" appears and clicking *OK* removes the window. This message appears both at the bottom of the *Update Average Daily Mass of Chemical Used* window and at the bottom of the *Specify Mass Balance Input Parameters* subtab.

Upon completion of Sequence A, B, C, or D, ChemSTEER recalculates equations EP4 through EP7 (unless the fix box is checked for any of these parameters, which causes that value to remain fixed), the mass balance update is completed, and the updated parameter values are displayed. If no warning message was displayed based on Sequence A, B, C, or D, ChemSTEER checks for any mass balance discrepancy as described in the <u>Entering/ Updating Mass Balance Parameters</u>, Type of Operation: <u>Continuous; Basis: Product</u> section of the User Guide and displays the result at the bottom of the Specify Mass Balance Input Parameters subtab.

## Calculation of a Non-default ADMUchem

A primary calculation for this operation is ADMUchem. The user has several options for calculating a non-default ADMUchem. These options are defined by the following conditions.

*Note:* You must follow the prescribed procedures to properly recalculate ADMUchem and other related parameters.

You should first check the fix boxes of any known parameters (up to three of the first five) and enter the known value(s) on the *Specify Mass Balance Input Parameters* subtab. If desired, you should then click the *Calculate* button next to the display box for the value of ADMUchem, which launches the *Update Average Daily Mass of Chemical Used* window.

In this window you have the option of retaining or updating the values of any of the parameters used in the equation shown. You may also check fix boxes for some parameters to set known values. Unchecked parameters may be adjusted by the previously described sequences.

After making appropriate updates, you may click the *Update Mass Balance* button, which launches the Electroplating Mass Balance Update Logic and Calculations listed below. Alternatively, if you click the *Restore Defaults* button, the ChemSTEER default values for all <u>changeable</u> parameters in *Update Average Daily Mass of Chemical Used* window appear.

If you click the *OK* button, the *Update Average Daily Mass of Chemical Used* window closes and ChemSTEER retains the values and fix box conditions last shown in the window. If you click the *Cancel* button, the *Update Average Daily Mass of Chemical Used* window closes and ChemSTEER retains the values and fix box conditions that first appeared in the window when it was launched.

At any time, clicking the *Calculate remaining parameters* button on the *Specify Mass Balance Input Parameters* subtab launches the Electroplating Mass Balance Update Logic and Calculations listed below.

## Electroplating Mass Balance Update Logic and Calculations

If the fix box for Yrinse is not checked, Yrinse =  $0.5 \times \text{Ybath}$ . If Yrinse is fixed and Ybath is changed, an error message will appear: "Would you like to update Yrinse to the default, Yrinse =  $0.5 \times \text{Ybath}$ ." Selecting Yes updates Yrinse and clears the Yrinse fix box.

ChemSTEER determines which of the following three conditions is true and proceeds to use the logic and calculations appropriate to the condition which is true.

Condition 1. ADMUchem is fixed or can be calculated by the standard mass balance logic (NS and OD or ADMUaddtv and Yaddtv are both fixed)

ADMUchem and the other associated parameters are fixed or calculated based on the relationships in equations EP2 and/ or EP5, as appropriate, completes any associated calculations that are possible using standard mass balance logic and calculations, and then launches the appropriate Sequence A, B, C, or D. These calculations complete the mass balance update.

Note: if OD is not fixed or is not calculable with standard mass balance equations (NS and ADMUchem are not fixed), 250 days per year will be assumed when calculating equation EP-2.

Condition 2. NS is fixed and neither OD nor ADMUchem are fixed (nor can ADMUchem be calculated by the standard mass balance logic (Yaddtv and ADMUaddtv cannot both be fixed for this condition))

## ChemSTEER calculates OD and ADMUchem using the following iterative approach.

- C2-1. OD = 1
- C2-2. ADMUchem is calculated using eqn. EP1
- C2-3. EPVop = ADMUchem x NS x OD
- C2-4. If EPVop < PVop and OD < 365 increase OD by one and repeat C2-2 and C2-3
- C2-5. ADMUchem = PV / NS / OD
- C2-6. Launch the appropriate Sequence A, B, C, or D

Condition 3. NS is not fixed and ADMUchem is not fixed and cannot be calculated by the standard mass balance logic (Yaddtv and ADMUaddtv cannot both be fixed for this condition)

## ChemSTEER calculates ADMUchem and NS based on the value of OD.

- C3-1 ADMUchem is calculated using equation EP1
- C3-2 NS is calculated using eqn. EP2

If NS is not calculated to be an exact integer, NS is set to the next highest integer. If NS had been calculated to be less than 1 (and then rounded up to 1 site) AND OD is NOT fixed, then OD is recalculated using EP2a.

C3-3 ADMUchem = PV / NS / OD

C3-4. Launch the appropriate Sequence A, B, C, or D

Fix Box(es) Selected	Condition	Equation Notes / Sequence (if non-standard)
No fix boxes selected	Initial Default Condition	Assume OD = 250, EP1, EP2, EP2a if NS was < 1, EP3, EP4, EP5, EP6, EP7
NS	Condition 2	EP4, EP5, EP6, EP7
NS and OD	Condition 1	EP3, EP4, EP5, EP6, EP7
NS and Yaddtv	Condition 2	EP5, EP6, EP7
NS and ADMUaddtv	Condition 2	EP5 (for Yaddtv), EP4 (for Yrm), EP6, EP7
NS and ADMUchem	Condition 1	EP2a, EP4, EP5, EP6, EP7
OD	Condition 3	EP4, EP5, EP6, EP7
OD and Yaddtv	Condition 3	EP5, EP4 (for Yrm), EP6, EP7
OD and ADMUaddtv	Condition 3	EP5 (for Yaddtv), EP4 (for Yrm), EP6, EP7
OD and ADMUchem	Condition 1	EP2, EP4, EP5, EP6, EP7
Yaddtv	Condition 3	Assume OD = 250 dpy, EP4 (for Yrm), EP6, EP7
Yaddtv and ADMUaddtv	Condition 1	EP5 (for ADMUchem), assume OD = 250 dpy, EP2, EP2a, EP3, EP4 (for Yrm), EP6, EP7
Yaddtv and ADMUchem	Condition 1	Assume OD = 250 dpy, EP2, EP2a, EP5, EP4 (for Yrm), EP6, EP7
ADMUaddtv	Condition 3	Assume OD = 250 dpy, EP5 (for Yaddtv), EP4 (for Yrm), EP6, EP7
ADMUaddtv and ADMUchem	Condition 1	Assume OD = 250, EP2, EP2a, EP5 (for Yaddtv), EP4 (for Yrm), EP6, EP7
ADMUchem fixed only	Condition 1	Assume OD = 250, EP2, EP2a, EP4, EP5, EP6, EP7
NS, OD, and Yaddtv	Condition 1	EP3, EP5, EP4 (for Yrm), EP6, EP7
NS, OD, and ADMUaddtv	Condition 1	EP3, EP5 (for Yaddtv), EP4 (for Yrm), EP6, EP7
Yaddtv, ADMUaddtv, and NS	Condition 1	EP5 (for ADMUchem), EP2a, EP3, EP4 (for Yrm), EP6, EP7
Yaddtv, ADMUaddtv, and OD	Condition 1	EP5 (for ADMUchem), EP2, EP3, EP4 (for Yrm), EP6, EP7
ADMUchem, NS, and Yaddtv	Condition 1	EP2a, EP5, EP4 (for Yrm), EP6, EP7
ADMUchem, NS, and ADMUaddtv	Condition 1	EP2a, EP5 (for Yaddtv), EP4 (for Yrm), EP6, EP7
ADMUchem, OD, and Yaddtv	Condition 1	EP2, EP5, EP4 (for Yrm), EP6, EP7
ADMUchem, OD, and ADMUaddtv	Condition 1	EP2, EP5 (for Yaddtv), EP4 (for Yrm), EP6, EP7

Operation Parameters tab / Shared Parameters/Factors subtab

When the Use of Electroplating Bath Additives operation is selected, the Shared Parameters/Factors subtab will display the Electroplating shared parameter/factor, "Electroplating Additive Type", by default. The user may change the Electroplating Additive Type default value by double-clicking on it in the table. The Electroplating default setting, as well as the available non-default option is summarized for the shared Electroplating Additive Type in the table below:

Shared Parameter/Factor	Default Value/Setting	Non-default Option
Electroplating Additive Type*	Organic Compounds	Suspended Solids

\* This parameter is shared by the EPA/OPPT Electroplating Rinse Water Loss Model and the EPA/OPPT Electroplating Spent Bath Disposal Model.

## Releases tab

For the *Changing Electroplating Bath* source/activity, the default model is:

• EPA/OPPT Electroplating Rinse Water Loss Model

For the *Rinsing Electroplated Parts* source/activity, the default model is:

• EPA/OPPT Electroplating Spent Bath Disposal Model

## Exposures tab

For the *Operating Electroplating Bath* source/activity:

- The overriding default for this worker activity: NWexp = 20 workers per site (Operating Electroplating Bath is the only default exposure activity).
- There is no default dermal exposure model.
- The default inhalation exposure model is the OSHA PEL-Limiting Model for Substance-specific Particulates (TWA or C).

As a default, the *Electroplating* generic scenario uses the OSHA PEL for chromium to calculate worker exposures. Therefore, the overriding default for KCk = 0.5 mg/m3 (chromium OSHA PEL) and Ypel = 0.25 (estimated chromium bath weight fraction). You may find additional OSHA values by clicking the *View Exposure Limits* button on the *Chemical* tab. Typical concentrations for various metal plating baths can be viewed in Chart B of the August 1996 *Generic Scenario: Electroplating* document.

## References

SAIC for US EPA/OPPT. <u>Generic Scenario: Electroplating</u>. August 1996.

# **RECIRCULATING WATER-COOLING TOWER ADDITIVE USE**

Revised March 30, 2004. This operation is applicable to the use of water treatment additives (e.g., as a scale, corrosion, or microorganism inhibitor) for recirculating cooling systems. The additives are transferred into the recirculating water to maintain a specified concentration. This operation estimates releases of the additive chemical as a result of the routine functions of the water-cooling system. The Summary Sheet: Recirculating Water-Cooling Tower (no date), was the primary reference source for the operation defaults described below.

It should be noted that the default usage rate for the additive is based upon the estimated daily releases of the additive. The daily releases are effectively calculated in the Mass Balance portion of the Operation Parameters tab instead of in the Releases tab. The release models for this operation use the values entered/calculated in the Operation Parameters tab.

## Operations tab $\rightarrow$ Description subtab

## Selected NAICS

There is no default NAICS code for this operation. Recirculating water-cooling towers are a general unit operation that may be found within virtually any industry sector. Therefore, the user must manually select an industry sector(s) relevant to their assessment.

## **Process Description**

NOTE: Release sources and exposure activities prior to the metering step of this operation (e.g., unloading of containers, empty container cleaning/disposal) are not included and must be manually selected. ChemSTEER's mass balance functions are not fully optimized to ensure an automatic balancing of chemical input to and output/release from an operation. For example, ChemSTEER does not currently account for pre-process releases of the chemical (e.g., as a result of amounts of the chemical remaining in transport containers). In operations where all of the chemical used is anticipated to be released (e.g., as in the Recirculating Water-Cooling Tower Additive Use operation), these pre-process releases will result in more of the chemical being released than is input to the operation. Future versions of ChemSTEER will include additional functions to correct for these pre-process releases.

The recirculating cooling tower additive containing the chemical being assessed is shipped to the sites in containers. Depending upon the facility's practice and the size of the shipping container, the additive may be unloaded into a storage tank until use or stored in the original container.

The additive is transferred into the recirculating water within the cooling tower at a specified rate, such that the desired concentration of the additive within the water is maintained. Losses of the additive primarily occur as a result of "blowdown" and "windage". Blowdown occurs when the facility must discard amounts of the water to adjust the concentrations of nonvolatile components (e.g., salts). Windage losses are a function of the equipment's mist eliminator design. If the additive is relatively volatile, evaporative losses to the air may also occur.

The default process description for this operation is as follows:

Unload water cooling-tower additive containing the assessed chemical from shipping container -> Store (optional) -> Mix into the cooling tower recirculating water to maintain a specific concentration (losses to blowdown and windage, and if the additive is volatile, to evaporation).

## Operations tab / Sources/Activities subtab

The following default source/activity is automatically listed on the Sources/Activities that will be assessed in the operation list on the Update Operation Sources/Activities screen (launched by the Update Sources/Activities button):

• <u>Recirculating Water-Cooling Tower Additive Releases</u> (Exposure - No, Release - Yes)

## **Available Activities**

• All other activities

NOTE: The *Recirculating Water-Cooling Tower Additive Releases* source/activity may not be used for any operation other than the Recirculating Water-Cooling Tower Additive Use operation.

## Operation Parameters tab / Mass Balance subtab

Clicking the Update Parameters button on the Mass Balance Parameters subtab launches the Update Operation Mass Balance Parameter screen. The following logic defines the default conditions and parameter values for this screen.

## Mass Balance Basis Selection tab

Default selections are *Continuous* and *Cooling Tower Additive Usage* (where Cooling Tower Additive Usage replaces Product since the basis is actually the additive used rather than a true product). The user cannot change these selections for this operation.

## **Specify Mass Balance Input Parameters**

ChemSTEER uses the parameters listed below and the following logic are used to perform mass balance calculations.

## Parameters

NOTE: The equivalent parameter designation in the Summary Sheet: Recirculating Water-Cooling Tower, if applicable, appears in parentheses.

DMIrm:	Daily mass input of raw material containing the assessed additive chemical
	(kg/site-day) (default: DMUaddtv)
DMIchem:	Daily mass input of the chemical in the raw material (assumed to be equal to the
	amount used) (kg/site-day) (default: DMUchem)
DMUaddtv:	Daily mass use of additive containing the assessed chemical (DMUaddtv
	replaces DMOprod for user-defined operations, but for the purpose of the mass
	balance is used in the same way) (kg/site-day) (default: DMUchem / Yaddtv)

DMUchem:	Daily mass of chemical in the additive used (DMUchem replaces DMOchem for user-defined operations, but for the purpose of the mass balance is used in the same way) (kg/site-day) (default: based on equations presented below)
Yrm:	Weight fraction of the chemical in raw material (0 < Yrm < 1; default: Yprod from previous operation or, if no previous value available, 1)
Yaddtv:	Weight fraction of the chemical in the additive (Yaddtv replaces Yprod for user- defined operations, but for the purpose of the mass balance is used in the same way) (0 < Yaddtv < 1; default: Yrm)
NS:	Number of sites (integer > 0) (default based on equations presented below)
OD:	Number of operating days (days/site-yr) (integer, 0 < OD < 365; default: 360)
Yctw (xR):	Weight fraction of the chemical in the cooling tower water (0 < Yctw < 1; default: 0.001)
Dctw:	Density of the recirculating cooling tower water (kg/gal) (0 < Dctw; default: 3.785 (equivalent to the density of water))
RRctw:	Recirculation rate of the cooling tower water (gallons/min) (0 < RRctw; default: 2,000)
HD:	Hours per day of cooling tower operation (hrs/site-day) (0 < HD < 24; default: 24)
DRRchem:	Daily recirculation rate of chemical in the cooling tower (kg/site-day) (0 < DRRchem) (default: based on equation presented below)
LFb:	Loss fraction of daily recirculation rate (DRRchem) for cooling tower blowdown $(0 < LFb < 1; default: 0.006)$
LFw:	Loss fraction of daily recirculation rate (DRRchem) for cooling tower windage (0 < LFw < 1; default: 0.001)
LFe:	Loss fraction of daily recirculation rate (DRRchem) from cooling tower evaporation (0 < LFe < 1; default: 0)

NOTE: The reference states that evaporative losses range from 0.5% to 3% of the recirculation rate. ChemSTEER defaults to 0 regardless of volatility. There is no method for determining the relationship between volatility and evaporative loss. If the assessed chemical has significant volatility, the user should make a judgment as to whether a non-zero value of LFe is appropriate.

These parameters are used to perform mass balance calculations on the ChemSTEER Operation Parameters windows as described by the default value calculations for this industry operation listed below. If the user chooses to update any default values, ChemSTEER updates other values using the logic and calculations described in the <u>Operation Parameters Tab</u>  $\rightarrow$  <u>Mass Balance Parameters Subtab</u> pages of the User Guide. Clicking the Restore defaults button will turn off the fix boxes set for any of the parameters, clear the values for all parameters on this screen, and replace them with the default values based on the logic and calculations listed below.

## **Default Calculations**

Default values for the mass balance parameters for this industry operation are calculated based upon the following logic and calculations.

- 1. DMUchem = (LFb + LFw + LFe) x DRRchem (see equation for DRRchem described below for the Daily Mass of Chemical calculations)
- 2. Yaddtv = Yrm = Yprod from the previous operation (or 1 if no previous operation)
- 3. DMUaddtv = DMUchem / Yaddtv
- 4. If PVop < DMUchem x OD, then NS = 1

If PVop > DMUchem x OD, then NS = PVop / (DMUchem x OD) ; if NS is not calculated to be an exact integer, it will be rounded up to the next highest integer above PVop / (DMUchem x OD).

- 5. OD (recalculated) = PVop / NS / DMUchem
- 6. DMIchem = DMUchem
- 7. DMIrm = DMIchem / Yrm

#### **Other Parameter Calculations**

A primary calculation for this operation is DMUchem (daily mass of chemical used). You may revise DMUchem by checking the fix box for DMUchem, which activates the *Calculate* button next to the display box for the value of this parameter. Clicking on this *Calculate* button launches the *Calculate* DMUchem: Daily Mass of Chemical Used (kg/site-day) window.

In this window, you have the option of choosing between two methods of calculating DMUchem. You may retain or update the values of any of the parameters used by the method that is selected. The first method, which is the ChemSTEER default, uses the equations:

DRRchem	= RRctw (recirculation rate of cooling tower water, gal/min) x Yctw (fraction of the chemical in the cooling tower water) x HD (operating hrs/day) x Dctw (density of the cooling tower water, kg/gal) x 60 min/hr
DMUchem	= (LFb + LFw + LFe) (sum of loss fractions for blowdown, windage, and evaporation) x DRRchem (daily recirculation rate of the chemical in the cooling tower, kg/site-day)

Each of the parameters used in the equations contain the default values shown in the parameter list above. You may change any values of the four parameters in the DRRchem equation and any of the three LF values and click the Recalculate button to recalculate values of DRRchem and DMUchem.

The second method allows you to fix DMUchem by checking the fix box next to the parameter. You may then change DMUchem and any of the three LF values and click the Recalculate button to recalculate value of DRRchem, which is recalculated using the following equation:

DRRchem = DMUchem (daily mass of chemical in the additive used, kg/site-day) / (LFb + LFw + LFe) (sum of loss fractions for blowdown, windage, and evaporation).

Clicking the *Restore defaults* button will clear the values for all parameters on these screens and replace them with the default values based on the information and logic listed above. Clicking Cancel will exit this window and retain the original value of DMUchem shown in the *Specify Mass Balance Input Parameters* screen. Clicking *OK* will exit this window and update the value of DMUchem in the *Specify Mass Balance Input Parameters* screen.

You may NOT directly enter a value for DMUchem in the *Specify Mass Balance Input Parameters* screen.

Changes to the value of DMUchem (via calculation in Method 1 or direct entry in Method 2 above) may cause the Number of Sites (NS) in the *Specify Mass Balance Input Parameters* screen to be recalculated (via Equation #4, above). If NS is fixed, ChemSTEER retains that value as a user-specified (fixed value) and re-calculates Operating Days (OD) (via Equation #5, above). Sometimes, the recalculated OD is an unrealistically low number or is greater than 365 (a warning message will appear that you will need to resolve).

If you receive this message and would like to update NS based on changes to DMUchem, click the *Re-calculate NS* button on the *Update DMUchem* screen. ChemSTEER temporarily sets OD = 360, re-calculates NS based on the new DMUchem and Equation #4 above, and then re-calculates OD based on the new NS using Equation #5. The *Re-calculate NS* button is only active when NS is fixed in the *Specify Mass Balance Input Parameters* screen.

### **Alternative Parameter Values**

The reference document contains several alternative parameter values and ranges for some parameters. If one or more alternative values apply to a particular assessment, you may consider changing the default values. These alternative values and ranges are summarized below.

Yctw should be selected based on the function of the additive within the cooling tower. The following table summarizes the default Yctw values in the reference document:

Function of the Cooling Tower Additive	Range in Concentration As Used (ppm)	Default Yctw (dimensionless)
Corrosion Control (default function)	50 to 1,000	0.001
Microorganism Control	1 to 20	0.00002
Scale Control	1 to 5	0.000005

The following table summarizes the default LF values in the reference document.

Source of the Release (Loss Fraction Designation	Range of Loss Fractions	Default LF (dimensionless)
Blowdown (LFb)	0.005 to 0.006	0.006
Windage (LFw)	0.00008 to 0.002	0.001
Evaporation (LFe)	0.005 to 3*	0**

\* Applicable to chemicals with volatility.

\*\* Applicable to non-volatile chemicals.

Finally, the reference document notes that large cooling towers have water recirculation rates (RRctw) of up to 100,000 gpm, and this value may be used to estimate conservative release estimates. The reference document indicates that a 2,000 gpm tower is a moderately-sized tower.

# Operation Parameters tab → Shared Parameters/Factors Subtab

When the *Recirculating Water-Cooling Tower Additive* operation is selected, the *Shared Parameters/Factors* subtab will display the Recirculating Water-Cooling Tower Additive shared parameter/factor, the amount of chemical to which a loss fraction is applied (Amt), by default. The Amt parameter is used by the three default release models of the default source/activity for this operation.

The default value for Amt is the value of DRRchem from the Mass Balance Parameters subtab. To change the value of Amt, you must recalculate DRRchem in the *Mass Balance Parameters* subtab by clicking the Calculate button next to the display box for the value of DMUchem. Clicking on this Calculate button launches the *Daily Mass of Chemical Used (DMUchem)* window, where DRRchem may be changed. You may NOT change the default value of Amt in the *Shared Parameters/Factors* subtab.

#### Releases tab

For the *Recirculating Water-Cooling Tower Additive Releases* source/activity, the following default models are pre-selected:

- EPA/OPPT Cooling Tower Blowdown Loss Model
- EPA/OPPT Cooling Tower Windage Loss Model
- <u>EPA/OPPT Cooling Tower Evaporative Loss Model (volatiles)</u> (activated <u>only</u> when AVPlow < VPchem)</li>

## Exposures tab

There are no default exposure models for the *Recirculating Water-Cooling Tower Additive Releases* source/activity.

#### References

Summary Sheet: Recirculating Water-Cooling Tower, No date.