11 Estimating Workplace Exposure and Industrial Releases Using ChemSTEER

The current version of ChemSTEER (**Chem**ical **S**creening **T**ool for **E**xposures and **E**nvironmental **R**eleases) and additional exposure-related information and resources are available at http://www.epa.gov/oppt/exposure/pubs/chemsteer.htm. This chapter will provide a brief summary of ChemSTEER. Please refer to the online resources for additional information.

11.1 What Does ChemSTEER Do?

ChemSTEER estimates workplace exposures and environmental releases of a chemical when specific measured values or monitoring data are not available. It provides screening-level estimates using worst case scenarios and input from other EPA methods and models.

11.2 How Does ChemSTEER Work?

As you enter the necessary information on your chemical and scenario(s) you "build" your assessment in ChemSTEER by entering these values:

- Data on the chemical to be assessed, including:
  - Production volume (or assessed volume) (kilograms per year)
  - Physical/ chemical properties (known or estimated)
- Select at least one operation (or work place scenario); options include:
  - Pre-defined industry-specific / use-specific operation
    or
  - User-defined operation.

Then you select at least one release source/ exposure activity within each operation. Each source or activity is associated with default models for calculating releases and worker inhalation and dermal exposures.

Next you enter mass balance and container-related data, review the models selected and the model input data, then run ChemSTEER.

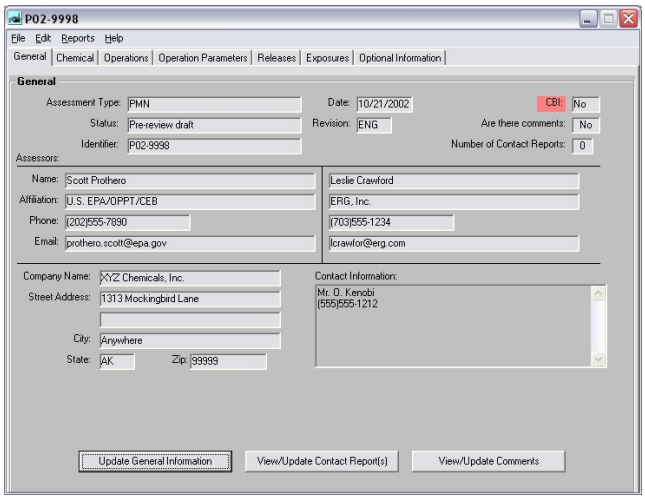
This chapter will summarize the entry screens or "tabs" in ChemSTEER, which are:

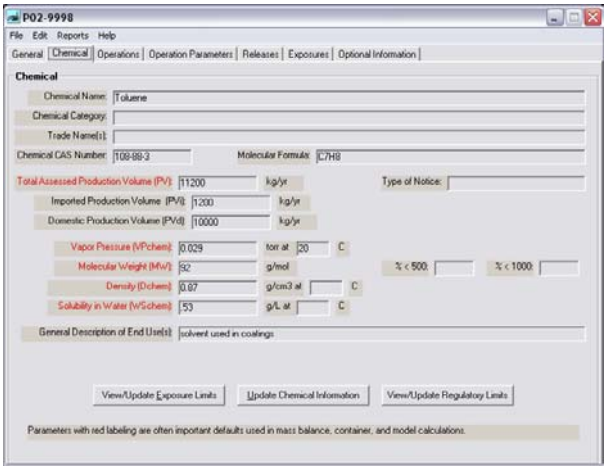
- General,
- Chemical,
- Operations,
- Operation Parameters,
- Releases,
- Exposures, and
- Optional Information.

11.2.1 The General Tab

This tab allows you to view and/or enter general information related to the ChemSTEER assessment, including:

- Assessment name,
- Date of completion,
- Assessor information,
- Contact information for the assessment,
- Report(s) summarizing information received from a contact, and
- General comments related to the assessment.





11.2.2 The Chemical Tab

This tab allows you to view and/or enter information related to the chemical to be assessed. The Production Volume (PV) (amount of chemical to be assessed) is an important input parameter because it is used in many mass balance, container-related, release, and exposure calculations.

The physical-chemical property parameters (e.g., vapor pressure, molecular weight) are needed by some release and/ or exposure models.

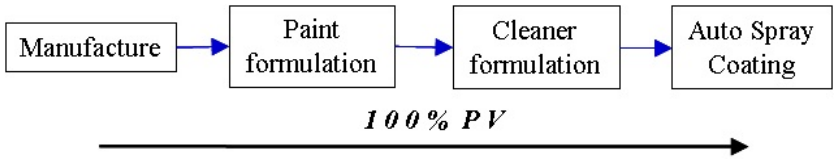
11.2.3 The Operations Tab

An operation in ChemSTEER is a work place or a set of "homogeneous" work places with essentially the same processes, equipment, chemical throughputs, procedures, and worker populations. Each work place within an operation is assumed to have the same chemical releases and worker exposures resulting from the chemical being assessed as the other work places within that operation. As you build the chemical assessment you select one or more operations in which the chemical is manufactured, processed, and/or used. Some examples of operations are:

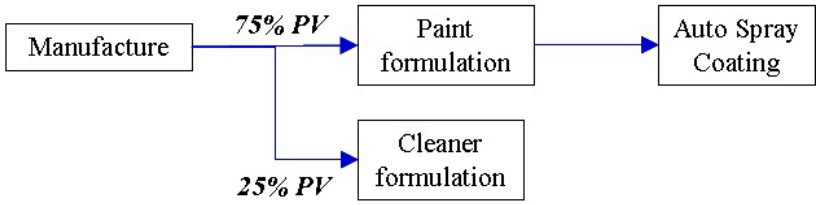
- Manufacture,
- Formulation of paint (User-defined Processing),
- Formulation of cleaner, and
- Automobile spray coating.

Operation Relationships Subtab

The relationships between multiple operations can be defined in ChemSTEER. A straight-series lifecycle of more than one operation (shown below) is the default relationship configuration.

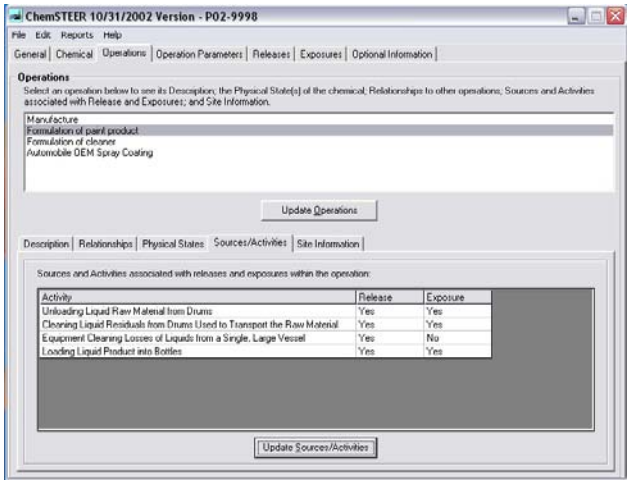


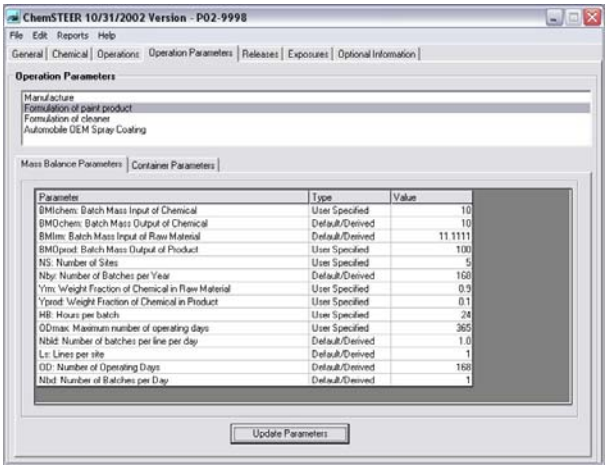
ChemSTEER allows you to re-define the operation relationships. For example, the series above can be rearranged into a more complex, branched lifecycle of operations shown below.



Sources/Activities Subtab

For each operation at least one release source or exposure activity (shown to the right) must be selected. This selection is critical, as it will determine which default release/exposure models are used for the calculations. A source/activity is a source of chemical release to the environment and/or an activity that results in a worker exposure to the chemical within an operation.



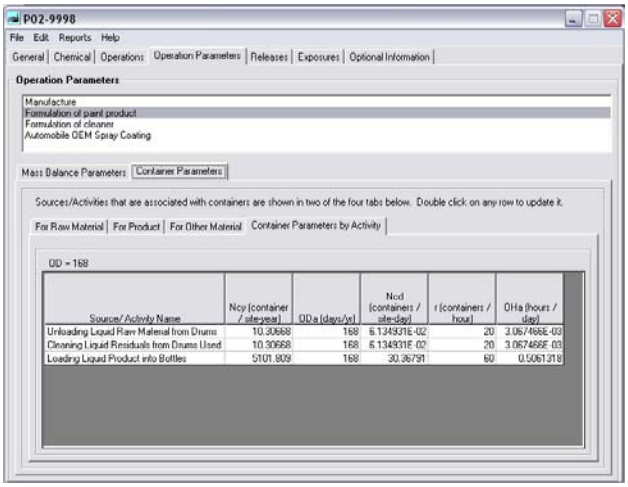


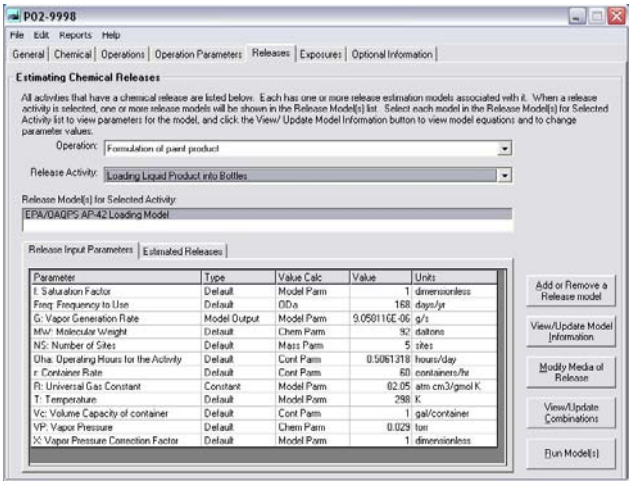
Mass Balance Parameters Subtab

Mass balance parameters (left) are the set of input values that define each operation and associated chemical throughputs. ChemSTEER allows you to enter the information that is known and will calculate remaining unknown parameters based upon a mass balance of the chemical around the operation. Consult the Help System to learn more about the logic by which ChemSTEER makes mass balance calculations.

Container Parameters Subtab

Container parameters (right) are the set of input values that define the number of containers that are filled with the chemical, emptied, and/or cleaned during each operation. As with the mass balance parameters, ChemSTEER allows you to enter information about the containers that is known and will calculate remaining unknown parameters based upon a mass balance.

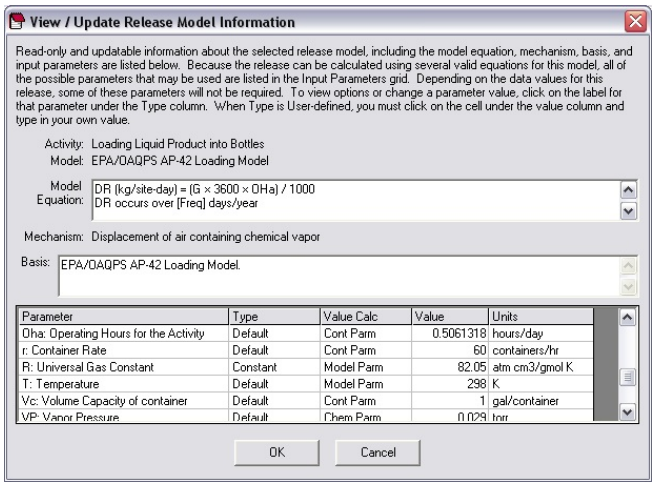




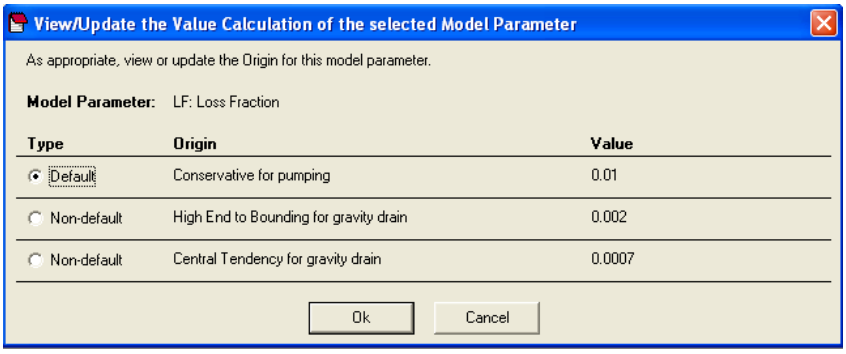
11.2.4 Releases Tab - Calculations

At least one default release model is associated with each source/ activity within each operation. The release models are used for calculating the chemical releases to the environment that occur during the activity. In the screen shown to the left, the default model for calculating releases from the 'Loading Liquid Product into Bottles' source within the 'Formulation of Paint Product' operation is the EPA/OAQPS AP-42 Loading Model.

Click on the "View / Update Combinations" button (shown in the previous image) and you can review the input parameters (shown on the right). Each release model contains the input parameter values that are necessary to perform the calculation by default. Some values are obtained via previous input or calculations (e.g., mass balance or container parameters) or are pre-programmed defaults. You may modify any of the model input parameters provided they are not determined through calculations performed in another input screen.



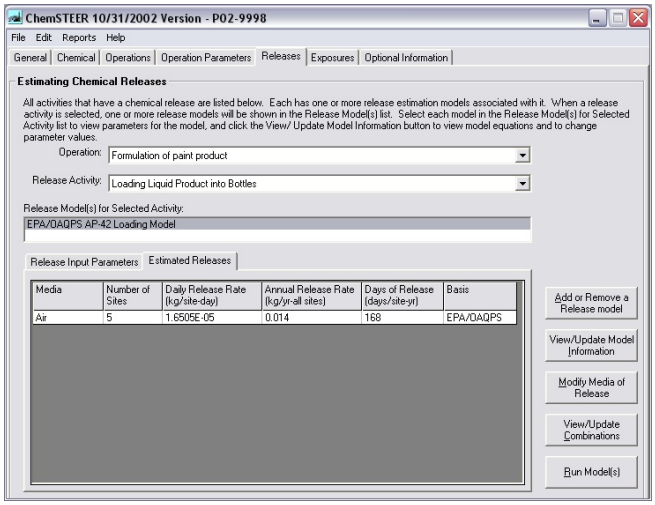
In the screen shown above you can also view the defaults and assumptions associated with the release model. The default assumptions are conservative and often represent "worst case".

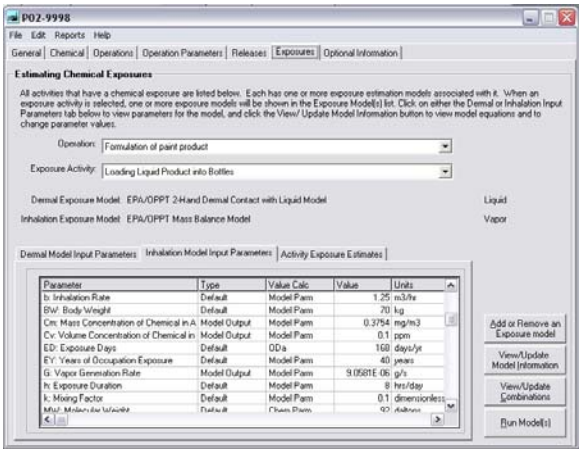


11.2.5 Releases Tab - Calculation Results

Environmental release results provided by ChemSTEER include:

- Media of release (I.e., air, water, incineration, and/or landfill),
- Number of sites releasing the chemical,
- Daily release rate (kg chemical per site-day),
- Days of release (days per site-year), and
- Annual release rate (kg chemical per year, all sites combined).

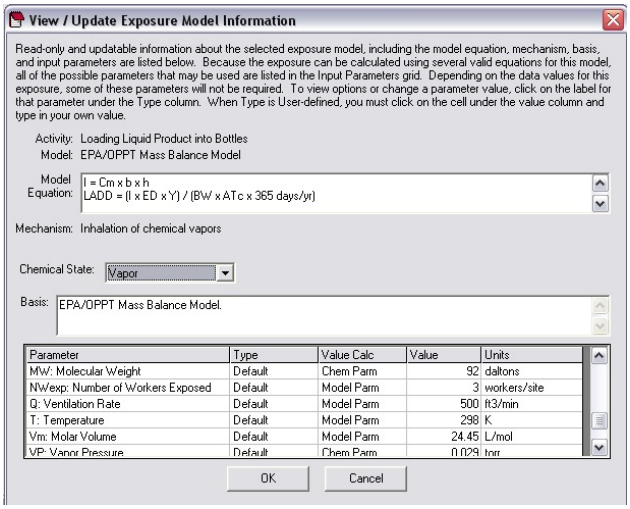


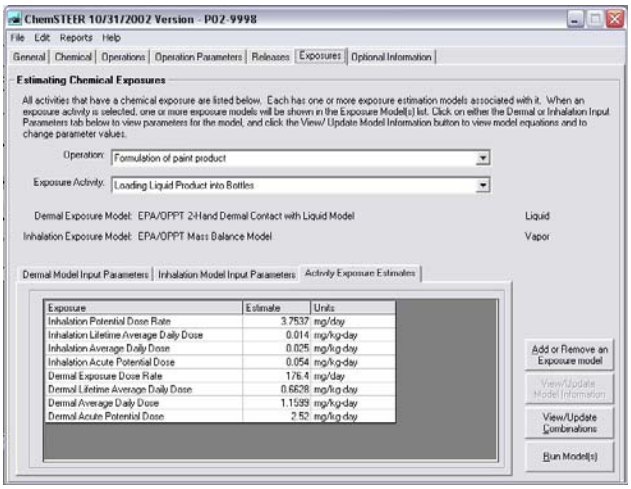


11.2.6 Exposures (Worker) Tab - Calculations

The exposure models in ChemSTEER are used to calculate the worker inhalation and dermal exposures to the chemical during the activity. As with the release sources, each activity resulting in a worker exposure will have associated default inhalation and/or dermal exposure model(s). In the screen shown to the left, the default inhalation model for worker exposure to the chemical vapor during the 'Loading Liquid Product into Bottles' activity within the 'Formulation of Paint Product' operation is the EPA/OPPT Mass Balance Model.

Each exposure model contains the input parameter values that are necessary to perform the calculation by default. Some values are obtained via previous input or calculations (e.g., container parameters, associated release model calculations) or are pre-programmed defaults. You may modify any of the model input parameters (provided they are not determined through calculations performed in another input screen).





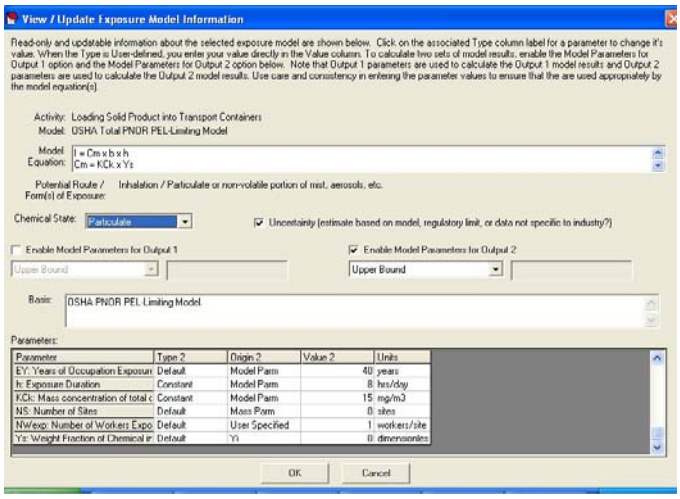
Exposures Tab - Calculation Results

Worker exposure results include the following estimates for both inhalation and dermal exposure:

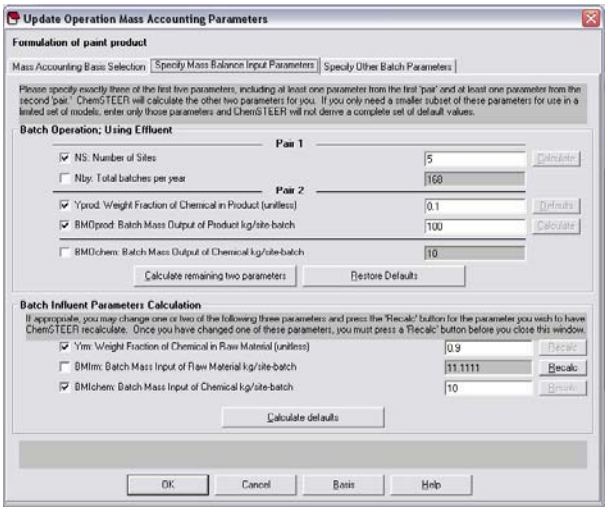
- PDR Potential Dose Rate (mg/day)
- LADD Lifetime Average Daily Dose (mg/kg-day)
- ADD Average Daily Dose (mg/kg-day)
- APD Acute Potential Dose (mg/kg-day)

11.2.7 Loading Solid Materials

The activity "Loading Solid Materials" is evaluated using the model OSHA PNOR (Particles Not Otherwise Regulated) PEL (Permissible Exposure Limit).



11.3 Features of ChemSTEER



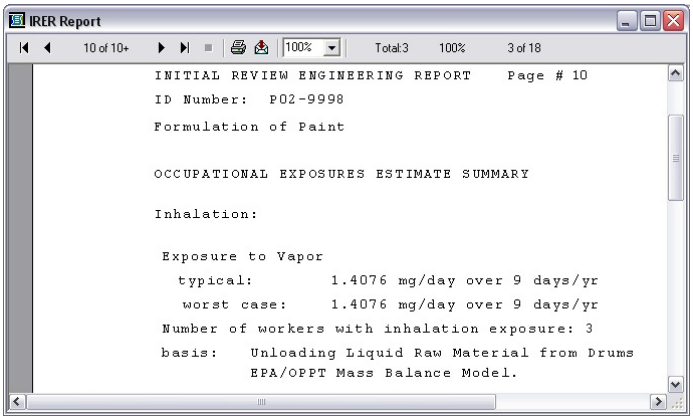
11.3.1 User-Friendly Design

ChemSTEER is designed such that new as well as experienced users can use the software to perform screening-level estimates. ChemSTEER walks you through the process of creating an assessment scenario.

Every screen has instructions that tell you what information must be entered before you proceed to the next screen. All default models are designed to be transparent and all assumptions and values are documented. ChemSTEER contains an extensive Help System that documents the bases for every model and every default value. The Help System also contains a library of background documentation.

11.3.2 Creating Summary Reports and Saving Assessments

You can view and print an EPA-formatted summary report (shown at the right). You can also export the report into various types of file formats (e.g., rich text format (.rtf)) to a choice of destinations on your hard drive or external disk. Assessments may be saved as individual records in a database file containing multiple assessments. Maintaining a database of multiple assessments allows you greater flexibility in organizing collections of assessments.



11.3.3 Next Version Expected Is Soon

The new version will have numerous enhancements from the current version. These enhancements include:

- A new release model (solid emission during dust handling),
- Improved Initial Review Exposure Report (IRER) generator,
- More flexible mass balance (don't have to enter all parameters),
- Several new inhalation models (roll coating mist, Auto Spray Coating (polyisocyanates)),
- Cooling tower water additive use operation and three associated models,
- Capability of opening and modifying assessments that were originally created and last saved using previous versions (after July 2003) of ChemSTEER,
- Revised number of worker calculation,
- Re-ordering the assessment sources/activities,
- Revised container parameters restore defaults, and
- Dual model output capabilities (including typical and worst-case for vapor models and small volume solids inhalation).

11.4 Running the Sample Chemical, Isodecyl Acrylate, in ChemSTEER

The following information about isodecyl acrylate will be entered in ChemSTEER

The sample chemical, isodecyl acrylate (CAS No. 1330-61-6), is a liquid that will be imported into the United States. Pure isodecyl acrylate will be used as a reactive diluent and processed to a 30% formulation for use in radiation curable coatings and adhesives, and related materials.

Pure isodecyl acrylate will be imported in transport containers at 11,200 kg/year, and delivered directly to the facility where it will be processed. For each batch (10 batches/year), isodecyl acrylate will be transferred directly into a single reactor and processed to a 30% formulation. Worker exposure will be prevented during transfer of pure isodecyl acrylate into the reactor via automated transfer equipment. Furthermore, a fugitive emissions capture device will be utilized to prevent release of isodecyl acrylate into the environment during transfer into the reactor. After formulation of each batch, the processed material will be transferred into the 55 gallon drums in which it will be transported to buyers. A single worker will be exposed by dermal contact and by inhalation during drumming. The reactor is cleaned once per year; occupational exposure will not occur during cleaning of the reactor. Releases to the environment will occur during drumming (fugitive releases to air) and cleaning of the reactor (fugitive releases to air and releases to surface water).

Screen captures showing the steps in entering isodecyl acrylate in ChemSTEER are not provided here. Readers can review Appendix G of this document which goes step-by-step through running ChemSTEER with another chemical.

Here are the results from running the sample chemical, isodecyl acrylate (CAS No. 1330-61-6) in ChemSTEER

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3/15/2005

INITIAL REVIEW ENGINEERING REPORT ID Number: Case Study
ENGINEER:      Thomas Webb \
PV (kg/yr): 11,200.00 Import
CBI: No

SUBMITTER: The Green chemical corporation
USE:     Reactive diluent in UV/EB curable coatings and adhesives.
OTHER USES:
MSDS: No Label: No

Gen Eqpt: gloves/goggles/glasses/local exhaust ventilation/general
mechanical ventilation/other (please specify): Respirator: air
purifying/organic vapor/dust/paint mist/supplied air/other (please
specify):
Health Effects: corrosive/flammable/other (please specify):
TLV/PEL: CRSS:
Chemical Name: Isodecyl acrylate
Chemical category: Acrylate
S-H20:   0.00303 g/L @ 25.00
VP:      0.0227000010 torr@ 25.00
MW:      212.34 %<500 %<1000
Phys state
NEAT: out of user-defined Processing: solution

consumer use:  No

SAT (concerns): Related cases:
Migration to groundwater: PBT rating: PBT
Health: Eco:

OCCUPATIONAL EXPOSURE RATING: NOTES & KEY ASSUMPTIONS:

POLLUTION PREVENTION CONSIDERATIONS

EXPOSURE-BASED REVIEW:     No    (0 criteria met)
1) # of workers exposed:   >1000? No
2)>100 workers with >10 mg/day inhalation exposure: No
3) (a)>100 workers w/1-10 mg/day inh. exp. &
>100 days/yr: No
(b)Routine Dermal cant: >250 workers &
>100 days/yr: No
```

3/15/2005

INITIAL REVIEW ENGINEERING REPORT CBI: NO

ID Number: case Study user-defined Processing Number of sites: 1

days/yr: 10
Basis:
Process Description:
ENVIRONMENTAL RELEASES ESTIMATE SUMMARY

Air
4.3040E-03 kg/site-day over 1 days/yr
from: Equipment cleaning Losses of Liquids from a single, Large vessel; Loading Liquid Product into Drums
basis: EPA/OPPT Mass Transfer coefficient Model.; EPA/OAQPS AP-42 Loading Model.

Air
9.6848E-04 kg/site-day over 9 days/yr from: Loading Liquid Product into Drums basis: EPA/OAQPS AP-42 Loading Model.

Water
11.2 kg/site-day over 1 days/yr
from: Equipment cleaning Losses of Liquids from a single, Large vessel
basis: EPA/OPPT sin le vessel Residual Model, CEB standard 1% res1dual.

OCCUPATIONAL EXPOSURES ESTIMATE SUMMARY Tot. # of workers: 1
Inhalation: Exposure to vapor
13.9353 mg/day over 10 days/yr
Number of workers (all sites) with inhalation basis: Loading Liquid Product into Drums; EPA/OPPT Mass Balance Model.

Dermal:

Exposure to Liquid at 30.00% concentration
529.20 mg/day over 10 days/yr

Number of workers (all sites) with dermal expo basis: Loading Liquid Product into Drums; EPA/OPPT 2-Hand Dermal contact with Liquids Model.

11.5 Entering Results from ChemSTEER in the Sustainable Futures Worksheet

EXPOSURE MODELS:			
INDUSTRIAL RELEASE AND EXPOSURE VALUES: CHEMSTEER			
Process	User-defined Processing	**Number of Release Days**	10
SIC Code / NPDES #		**Number of Facilities**	1
Occupational Exposure Values			
	Cancer LADD	**Chronic ADD**	**Acute APDR**
Dermal	0.118 mg/kg-day	0.207 mg/kg-day	7.56 mg/kg-day
Inhalation	3.12×10^{-3} mg/kg-day	5.45×10^{-3} mg/kg-day	0.199 mg/kg-day
Environmental Release Values			
Release to Water		11 kg/year (11 kg/site-day over 1 day/yr)	
Release to Air (Fugitive) [drumming]		0.0097 kg/year (9.7×10^{-4} kg/site-day over 10 days/yr)	
Release to Air (Fugitive) [reactor cleaning]		0.0033 kg/year (3.3×10^{-3} kg/site-day over 1 day/yr)	
Release to Landfill			
Release from Incineration			
Other Release Activities			

EXPOSURE MODELS:			
INDUSTRIAL RELEASE AND EXPOSURE VALUES: CHEMSTEER			
Process	User-defined Processing	**Number of Release Days**	10
SIC Code / NPDES #		**Number of Facilities**	1
Occupational Exposure Values			
	Cancer LADD	**Chronic ADD**	**Acute APDR**
Dermal	0.118 mg/kg-day	0.207 mg/kg-day	7.56 mg/kg-day
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Release to Landfill			
Release from Incineration			
Other Release Activities			