



Consumer Exposure Model

Consumer Exposure Model (CEM)

DRAFT User Guide

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Note to Peer Reviewers

OPPT aims for CEM to be a flexible, user-friendly, and scientifically rigorous tool to rapidly screen exposure to consumer products and articles across a range of exposure scenarios and pathways. To this end, OPPT wishes to solicit feedback on both the performance and ease of use of the tool. The scenarios, chemicals, and defaults currently included in CEM are based on available data and professional judgment and are present in order for model users to have the ability to use all parts of the model. At any time, defaults, chemicals, or use scenarios could be deleted, added, or refined based on feedback received during beta testing, peer review, or newly available information.

CEM retains six existing models from the E-FAST model and adds nine additional models. The updated version now includes six inhalation models, five ingestion models, and four dermal models. All CEM models are used to estimate chemical concentrations in exposure media, including indoor air, airborne particles, settled dust, and soil. The models also evaluate dermal flux of a chemical through the skin and the migration of a chemical from an article to saliva. These are combined with media contact rates and various exposure factors to determine the single daily dose and chronic average daily dose of chemical resulting from product and article use scenarios associated with 85 product and article categories. Additionally, the model is parameterized for a variety of indoor use environments, including residences and specific rooms within residences, offices, schools, automobiles, and limited outdoor scenarios.

Notably, models to estimate exposure to semi-volatile organic compounds (SVOCs) from consumer articles have been incorporated, including a mass balanced model for estimating emissions and indoor fate and transport of SVOCs. Inhalation of airborne gas- and particle-phase SVOCs, ingestion of previously inhaled particles, dust ingestion via hand-to-mouth contact, ingestion exposure via mouthing, and direct and gas-to-skin dermal exposure of SVOCs are incorporated.

The latest version of CEM also has the option to model higher exposure associated with product use near the breathing zone. The option, called the “near field option” creates a small personal breathing zone around the user during product use in which concentrations are higher, rather than employing a single well-mixed room. This option should be applied with discretion as it is better used for product use categories associated with stationary rather than mobile use.

Additionally, CEM has been developed to be a flexible tool that can assess both data-rich and data-poor chemicals. CEM requires that the chemical molecular weight, vapor pressure, K_{ow} , and K_{oa} be provided. These values can be estimated from EpiSuite™. All other input variables, including mass transfer, partition, and diffusion coefficients can either be estimated within CEM from these baseline physical-chemical parameters and model defaults or, if data are available, can be supplied by the modeler.

Based on the feedback of the Beta reviewers, the following changes have been implemented in CEM:

1. Activity patterns were revised to capture mostly stay-at-home, part-time out-of-the home (daycare, school, or work), and full-time out-of-the-home residents.
2. A model considering ingestion of inhaled particles that are trapped in the upper airway was added.
3. An option to use products outdoors was added.
4. The dermal exposure from articles model was revised to reflect CONSEXO approach and data from the OPP Residential Scenarios.
5. The product applied to the ground outdoors model was revised to account for multiple product applications.

6. The dermal exposure model for air-to-skin transport was revised to include a steady-state flux from the air to the skin.
7. The option to specify a fraction absorbed, in addition to an absorption constant, was added to the dermal exposure models.
8. Multiple options to increase the user-friendliness of the model and decrease model run-time were added, including additional help screens, default parameters, parameter estimators, search functions, and code refinements.
9. Multiple options for naming, outputting, formatting, and saving reports were added.

These changes result in an update from CEM beta version 1.3 sent for beta testing in Fall 2015 to CEM beta version 1.4 sent for peer review in June 2016. Version 1.4.1 is identical to version 1.4 with one exception. An error was corrected that did not allow for user-defined chemicals to be matched with user-defined physical-chemical properties. In version 1.4.1, user-defined (as well as prepopulated) chemicals and associated physical-chemical properties can be analyzed. Following incorporation of peer review comments, Version 2.0 of CEM is expected to be posted by the end of calendar year 2016.

Introduction

Under the Toxic Substances Control Act (TSCA), the U.S. Environmental Protection Agency's (EPA) Office of Pollution Prevention and Toxics (OPPT) assesses potential exposures of new and existing chemicals. When evaluating chemical uses, OPPT uses available measured data together with modeling tools to provide scientifically based estimates of exposures and doses.

This guidance document describes the Consumer Exposure Model (CEM), which OPPT developed to estimate human exposure to chemicals contained in consumer products and articles:

Products are generally consumable liquids, aerosols, or semi-solids that are used a given number of times before they are exhausted.

Articles are generally solids, polymers, foams, metals, or woods, which are always present within indoor environments for the duration of their useful life which may be several years.

Although there are existing definitions of consumer products and articles, they are distinguished from each other in a more general way here. Certain chemicals may only be added to articles, others only used to formulate products, and others could be used for both. For the purposes of exposure assessment, products and articles are treated differently. Formulations, anticipated use patterns, and available approaches to estimate exposure are different.

CEM was originally developed as a module within EPA's Exposure and Fate Assessment Simulation Tool (EFAST). Compared with the original version, the updated version contains all existing models but also evaluates a wider range of products and articles, use scenarios, and exposure estimation methods. The updated CEM can assess exposures from:

Inhalation – from vapors emitted from products that are sprayed, products that applied to surfaces, products placed in a room, products that are added to water, and to vapors and particulates containing SVOCs from articles present within an indoor environment;

Non-Dietary Ingestion – to chemical adsorbed to dust or soil or present on the surface of articles and incidentally ingested through mouthing, swallowing, or hand-to-mouth contact; and

Dermal contact – to liquids present on skin after using consumer products, transfer of residue from the surface of articles, and transfer from vapor-phase air to skin.

CEM includes several distinct models appropriate for evaluating specific product and article types and use scenarios. For example, models for products recognize that emissions are generally highest for a shorter period of time during use(s), and generally lower or non-existent when products are not being used. Product-use models include exposures from direct use and/or close proximity. Models for articles assess migration of additive chemicals out of the articles and subsequent exposure through ingestion of dust particles, inhalation of vapor-phase or particle phase chemicals in the air, mouthing of chemicals present on an article's surface, dermal absorption through skin contact, or mouthing of chemical's present on hands or other parts of the body after contact with articles.

Product use categories define various kinds of products. Examples include aerosol spray paints, laundry detergent, foam-based furniture, hard-plastic toys, and motor oil. Chemicals are present in products for many different reasons. The reason why a chemical is included in a product—its specific job—is referred to as its functional use. Examples include propellants, flame retardants, solvents, surfactants, plasticizers, and repellants. Functional uses are important to help define generic formulations within a product or article category. Harmonized nomenclature of product and article use categories along with functional use categories can help inform exposure scenarios over time through development of generic formulations which provide typical weight fraction values or ranges that a given chemical is present.

Exposure scenarios combine information needed to estimate consumer exposures for a given product use. A product use category can vary in specificity of the product and its application. An exposure scenario developed for a specific product use category will have a scope focused on activities with a common exposure source and associated parameters. Exposure scenarios contain documented information needed to perform exposure calculations, including:

- Formulations (e.g., weight fraction),
- Use patterns (e.g., frequency, duration, and amount used),
- Human exposure factors (e.g., body weight, inhalation rate),
- Environmental conditions (e.g., air exchange rates and room size), and
- Chemical or product-specific properties (e.g., product density, vapor pressure, molecular weight, diffusion coefficient, overspray fraction, transfer factors, dilution factor).

Default values are available, but the model can be run with user-defined inputs as well. **The use of measured values informed by current and robust collection of exposure data is preferred.**

The models within CEM are deterministic and appropriate for use in **screening level assessments**. Variation has been incorporated (high, moderate, and low choices) for many of the parameters which allow for estimation of central tendency and reasonable worst case exposure estimates. Chemicals can be used in many different ways. How much of a product is used (amount), how often (frequency), and for how long (duration) vary. This information, when combined with human and built environment exposure factors, can be used for screening level exposure assessments. For articles, additional information on diffusion rates and other physical-chemical properties are needed to estimate emissions and subsequent exposures. Higher-tier models such as CONSEXPO, MCCEM, IAQX, iSVOC, and CONTAM provide more robust estimates of exposure, including probabilistic ranges, but also require measured data such as emission rates from chamber studies. See Section 3 for a detailed discussion of the individual consumer exposure models contained within the CEM and associated data requirements.

This guidance document contains information previously included in the Consumer Exposure Module of E-FAST's User Guide, and information previously included in the AMEM polymer migration model. To the extent possible, this information has also been incorporated directly into the model through use of help screens.

The contents of this user guide include the following:

- Directions for downloading and operating CEM

Summary of models contained within CEM (including domain scenarios and chemicals)
Detailed equations and description of models contained within CEM
Areas for future enhancement
Appendix of definitions of model parameters used in CEM
Appendix of model inputs used in CEM

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1. Downloading and Operating CEM

To use CEM, you will need to save three program files to your computer. These include a Microsoft Access database file, which is the main CEM program file, and two “executable files” that support the main program file. You will not use the executable files directly, but they must be present in the same folder location as the main CEM program file for the model to function.

The main program file and the executable files are provided together in a “zip” file (i.e., a file format commonly used for compression and transmission of large computer files).¹ You must “unzip” the CEM files before the first use. CEM will not run if you attempt to open and use it from within the zip file (i.e., without unzipping the CEM files). The CEM files may be unzipped to a computer hard drive, network folder, or other storage location. For best performance, it is recommended to unzip CEM to your computer hard drive. Follow the steps below to download, unzip, and open CEM.

1. Download zip file titled “CEM Version XX.zip” to your hard drive or other storage location (see above). You may need to copy or move the file from “downloads” into the folder location of your choice. Opening CEM without first saving the zip file may result in errors.
2. Right click on file and select “Extract All” or “Extract to here” or similar command. The specific command to unzip/extract the file may differ depending on which file compression utility you use (e.g., WinZip, 7-zip).
3. Click “Extract”. A new folder will appear where you downloaded the original zip file.
4. Double click the folder to open it and double click the main CEM file titled “CEM Version XX.accdb”.
 - a. This folder also includes a copy of this User Guide and two executable files (CEM_NFFF_v25.exe and SVOC10_v7.exe).
5. The first time you open the main CEM file, Windows security will disable the model code. You must click “Enable Content” near the menu bar at the top of the screen to enable the model programming to run.
6. At the top right of the screen, to the right of the CEM logo, select ‘View a Saved Analysis’ or ‘New Analysis’ to begin.

Overview

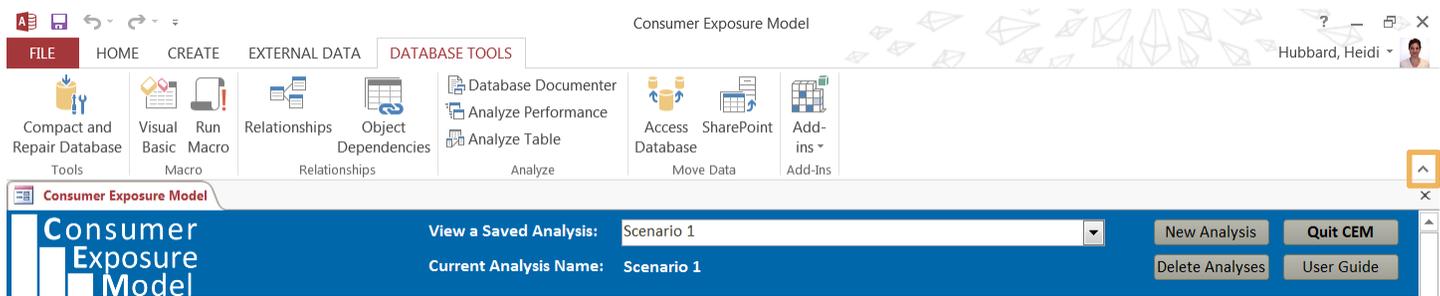
CEM is organized within Microsoft Access with a heading bar containing application-wide commands, and tabs for entering required inputs, running the model, and viewing results. CEM has the following tabs:

1. Scenario
2. Inputs
 - a. Chemical Properties
 - b. Product/Article Properties
 - c. Environment Inputs
 - d. Receptor Exposure Factors
 - e. Activity Patterns
3. CEM Models
4. Results
5. Lookup Tables

Instructions for walking through the heading bar and each of the tabs are described in the following sections. Definitions of terms and parameters are included in the glossary and the detailed descriptions in Section 3 include more discussion of certain model parameters.

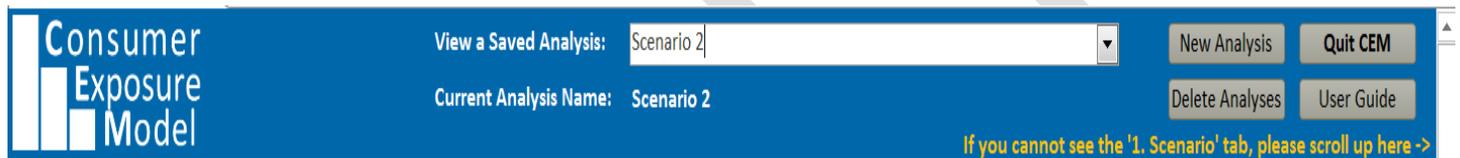
¹ You will need a file compression/archival utility to open the zip file. Several free compression utilities are available, and many new computers come with a compression utility pre-installed. Examples common compression utilities include WinZip and 7-Zip.

Hiding Access Task Bar



When CEM is opened, the Access Taskbar (that includes, File, Home, Create, External Data, and Database Tools and subheading options underneath each) is automatically visible. These controls are not used by CEM. To hide these and maximize CEM viewing, click the “up” carot on the bottom right side of the Access Task Bar. This action will need to be taken only upon opening CEM.

CEM Heading Bar



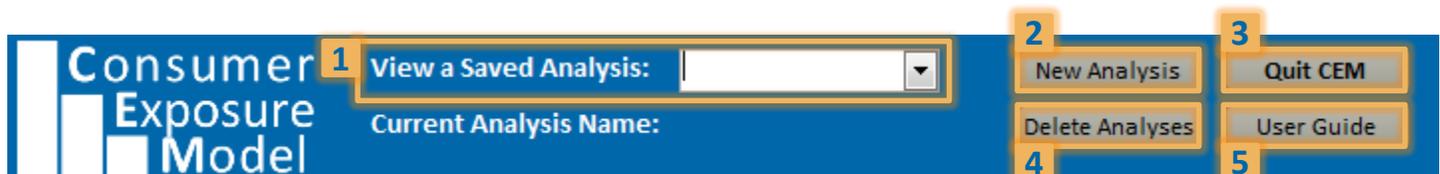
When CEM is opened, all controls beneath the heading bar are locked. To begin using CEM, first choose either:

1. A previously saved analysis or
2. Create a new analysis. A new analysis can be created based on CEM default inputs or inputs saved from another analysis.

Additional controls on the heading bar include:

3. The 'Quit CEM' button closes CEM. All selections within CEM will be saved automatically.
4. Use the 'Delete Analyses' button to delete one or more previously saved analyses.
5. The 'User Guide' button provides help on specific CEM inputs, and allows browsing by topic or text searching.

CEM is built in Microsoft Access. As a default, Access orients to the bottom of a tab. To see the entire contents of a tab, use the scroll bar to return to the top. A note to this effect is included on the heading bar.



1. Scenario tab

1. Scenario	2. Inputs	3. CEM Models	4. Results	Lookup Tables	
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This tab includes basic information about the exposure scenario, and choices made on this tab affect which inputs will be required for the remaining tabs. Scenario features specified on the Scenario tab include:

- 1. Chemical of Interest** – Choose an existing chemical, or add a new one. The “Filter” option can be used to search the chemicals pre-populated in CEM by text string or CAS.
- 2. Product or Article Used** – Choose a product or article, and choose whether or not to use the default use environment for that particular item. When a product/article is selected, CEM pre-populates with known default values, pre-selects the applicable exposure models, and identifies required inputs. A wide range of product and article categories is provided that should cover the range of expected uses. However, in the event that a product or article is not explicitly included, an existing category could be adapted noting that product- or article-specific defaults would need to be adjusted and are not provided up front as defaults. In the previous version of CEM, this was a "user-defined" scenario.
- 3. Product User(s) and Receptor(s)** – CEM may be run for multiple product users and receptors including adults, youths (aged 11-20 years), and children (aged 1-10 years). A product user is defined as receptor who uses a product directly. A receptor is a non-product user who is incidentally exposed to the product or article. Some products may be used more typically by adults and/or by children. The model user should carefully consider who is likely to use a given product when making this choice. Choices about whether the users typically spend most of their time at their residence, school, or other non-residence environment determine default activity patterns.
- 4. Activity Patterns** – CEM is populated with three activity patterns. One in which the receptor primarily spends time within the home; one in which the receptor works or attends school out of the home part-time; and one in which the receptor works or attends school out of the home full-time. The activity patterns were developed based on Consolidated Human Activity Database (CHAD) data of activity patterns and are detailed on the Activity Pattern tab.
- 5. Use Environment** – The room or other location where the product/article is used. Choose from the existing pick-list options, and select only one environment for a given scenario. Additional options are available in subsequent tabs to edit the default values pre-populated for the use environment.
- 6. Weight Fraction of Chemical in Product/Article** – If the selected scenario calculates exposure from the use of a product or presence of an article, enter the level of chemical in the product initially.
- 7. Initial Concentration of SVOC in Article** - If the selected scenario calculates exposure from the presence of an article, either enter the level of chemical in the article initially or use the estimator button to calculate the initial concentration from the weight fraction and density.
- 8. Background Air and Dust Concentrations** – In order to quickly compare exposure attributed to consumer products and articles to background exposures, a user-defined background air and dust concentration can be specified. The chronic exposure to these media are calculated and reported separately from pathway-specific exposures. These are set to zero as default.
- 9. Scenario Description/Notes** – An optional free-text field to enter a scenario description for later reference.
- 10. Modeling Options** – Options provided for relevant models (models that do not apply will appear gray). Choose the appropriate options pertaining to emission rate, near-field zones, and dermal absorption, as applicable. Further information can be found in the model descriptions in Sections 2 and 3.
- 11. Models for the Selected Product or Article** – This menu lists the models that apply to the selected product or article and a general indication of the domain of applicability as denoted by VOC, SVOC, or SVOC/VOC.

12. Help Buttons – Clicking the mouse on a question-mark button will show a help screen with instructions for each feature.

2. Inputs tab

The Inputs tab is where details such as chemical properties and product use details are entered. The Inputs tab includes five subtabs (“a” – “e”), each of which is described below.

Because CEM includes several distinct models, not all inputs are required for every scenario. CEM automatically identifies inputs required for the current scenario and disables unneeded inputs. Required inputs can be identified by labels with blue text; inputs that are not required have gray labels and input boxes and may not be entered for the current scenario.

CEM is pre-populated with default values associated with chemicals, products and articles, and receptors. In many cases, high, medium, and low defaults are provided. The user should exercise caution when selecting defaults to ensure that the scenario modeled is reasonable. Any defaults in CEM may be overwritten by the user. CEM includes a “Restore All Default Inputs” button along with the five subtabs. If this button is selected, the defaults are restored across all five tabs. Inputs that are not populated by a default are reset to blank.

2.a. Chemical Properties Input tab

The Chemical Properties Input tab includes information on the physical-chemical properties of the chemical-of-interest chosen in the Scenario tab. Examples include:

Vapor pressure,
 Molecular weight,
 Saturation concentration in air,
 Water solubility,
 Henry's Law coefficient
 Octanol-air partition coefficient, and
 Octanol-water partition coefficient.

Additionally, this tab contains data on the parameters required to estimate emissions from articles and transfer to dust. More details concerning these parameters and how they are incorporated into CEM are presented in the Section 3 description of model INH06. Examples include:

Solid-phase diffusion coefficient,
 Partition coefficients between air and dust, TSP, sources, and interior surfaces (sinks), and
 Mass transfer coefficients to TSP, dust, and interior surfaces (sinks).

When estimating chemical exposures, measured data are preferred over estimates whenever available. Because measured data are often unavailable, however, estimation tools are available for several inputs. For chemicals within the domain of the training sets used for QSAR development, EPA recommends the use of EPI-Suite Version 4.11 ([U.S. EPA, 2012a](#)) to estimate physical-chemical properties if empirical data are not available.

CEM incorporates many parameter estimators in the Inputs subtabs. To explore a parameter estimator, click on the "Estimate" button. This will provide background on the parameter, the estimator equation, equation inputs, and the estimated parameter. Click "Copy to Form" to close the estimator and paste the estimated parameter to the Input tab. To estimate all parameters on a tab at once, click the "Estimate All" button. This will not show the individual estimator equations.

All properties required by CEM are shown on the chemical properties tab, even though not all properties are required by each model. Properties not required by the model selected are presented in gray and are inactivated.

1. Click the 'Estimate' button next to an input field to use an estimator.

1. Scenario 2. Inputs 3. CEM Models 4. Results 5. Reports

a. Chemical Properties b. Product/Article Properties c. Environment Inputs d. Receptor Exposure Factors e. Activity Patterns

Values initially shown are default values. Override the default values by using the picklist or entering user-defined values.

Chemical Property/Attribute		Estimate All
Chemical Name:	Phosphoric acid, triphenyl ester	
CAS No.:	115866	
Vapor Pressure (torr):	0.00000628	
Molecular Weight (g/mol):	Required 326.2865	1 Estimate
Saturation Concentration in Air (mg/m3):	1.10e-01	
Log Octanol-water Partition Coefficient (-):	4.59E+00	
Log Octanol-air Partition Coefficient (-):	8.46E+00	
Water Solubility (g/100g water):	Not Required	
Henry's Law Coefficient (atm/M):	3.31E-06	

2.b. Product/Article Properties Input tab

1. Scenario	2. Inputs	3. CEM Models	4. Results	Lookup Tables	
a. Chemical Properties	b. Product Properties	c. Environment Inputs	d. Receptor Exposure Factors	e. Activity Patterns	

The Product/Article Properties Input tab is used to enter required inputs. Default values are available for many inputs and non-default values can be entered for most inputs. Not all information is required for all models. Inputs required by the model(s) applicable to the selected product or article are highlighted in blue text and must be entered before moving to the next tab.

2.c. Environment Inputs tab

1. Scenario	2. Inputs	3. CEM Models	4. Results	Lookup Tables	
a. Chemical Properties	b. Product Properties	c. Environment Inputs	d. Receptor Exposure Factors	e. Activity Patterns	

Use the Environment Input tab to enter required inputs about the environment(s) where the product or article is used. Default values are available for many inputs and non-default values can be entered for most inputs. Not all information is required for all models. Required inputs are highlighted in blue text and must be entered before moving to the next tab.

2.d. Receptor Exposure Factors Input tab

1. Scenario	2. Inputs	3. CEM Models	4. Results	Lookup Tables	
a. Chemical Properties	b. Product Properties	c. Environment Inputs	d. Receptor Exposure Factors	e. Activity Patterns	

The Receptor Exposure Factors Input tab is used to provide information on product or article users and incidentally exposed humans. All exposure factors are presented by receptor age group.

1. Required exposure factors are listed in the box on the left.
2. The box on the right shows the values for the factor selected to the left.
3. Default values are shown alongside the values entered for the current analysis.
4. Enter non-default values for the specific analysis under Analysis Value. For SA-BW (skin surface area to body weight) Ratio exposure factors, a drop-down menu is provided for low, medium, and high estimate values. An additional table presents SA-BW Ratios for differing areas of skin exposure (e.g., whole body versus both hands.)

Choose an Exposure Factor 1

- Body Weight (kg)
- Exposure Duration - Chronic (years)
- Exposure Duration - Acute (days)
- Averaging Time - Chronic (years)
- Averaging Time - Acute (days)
- Inhalation Rate During Use (m3/hr)
- Inhalation Rate After Use (m3/hr)
- SA-BW Ratio

Receptor-specific Exposure Factors Values for this Analysis

Receptor	Default Value	Analysis Value
Adult (≥21 years)	80	80
Youth (16-20 years)	71.6	71.6
Youth (11-15 years)	56.8	56.8
Child (6-10 years)	31.8	31.8
Small Child (3-5 years)	18.6	18.6
Infant (1-2 years)	12.6	12.6
Infant (<1 year)	7.8	7.8

Restore Defaults

2.e. Activity Patterns Input tab

1. Scenario
2. Inputs
3. CEM Models
4. Results
Lookup Tables

a. Chemical Properties
b. Product Properties
c. Environment Inputs
d. Receptor Exposure Factors
e. Activity Patterns

CEM employs three default activity patterns, one corresponding to a person who spend most of their time at home, one corresponding to a person who works or attends school part of the day, and one corresponding to a person who works or attends school all day. These activity patterns are presented for reference on the Activity Patterns tab. Only one activity pattern can be selected for all receptors for a single model run in CEM.

For receptors who are also product users, the activity pattern for the day of use that places the receptor in the use environment for the greatest period of time will be selected by CEM. For example, if a product is selected for use in the home, the user will follow the Stay-at-Home activity pattern during a product use day, regardless of their activity pattern selected for non-use days. A receptor that uses a product in the office will follow the Full-Time-Work activity pattern for the product use day. Additionally, the use-day activity pattern will be overridden to place the user in the room of use beginning at the Use Start Time specified. The user will remain in the room of use for the duration of product use selected. The start time and duration of use should be selected so that product use occurs within one 24-hr day. This logic applies only to product use, not article exposure.

3. CEM Models tab

1. Scenario
2. Inputs
3. CEM Models
4. Results
Lookup Tables

Model Selection
INH-01
DER-01a

Click the CEM Models tab after completing the Scenario and Inputs tabs. This tab allows users to review the scenario and input selections and to run the applicable exposure models.

1. The Model Selection subtab summarizes the models applicable to the selected product or article. These models are selected by CEM and cannot be edited.
 - a. The Model Selection sub-tab includes an option to save intermediate estimates when running inhalation models INH01-INH06. Intermediates estimates include emission rates, contaminant concentrations in air, and cumulative

1. Scenario
2. Inputs
3. CEM Models

1
Model Selection
INH-01
DER-01a
2

chemical intake by each receptor. For the chronic and acute assessments, these intermediate estimates are shown for each 30-second time step for the first 24 hours (i.e., the day of product use). For the chronic assessment only, hourly intermediate estimates are presented from the beginning of the second day through the remainder of the 60-day modeling period. The 60-day modeling period is used to calculate the total exposure associated with a single use of a product. Choosing not to save intermediate estimates will allow the model to run more quickly. Chronic and Acute exposure estimates are always presented whether or not intermediate estimates are saved.

- b. After reviewing inputs, click the 'Run CEM Models' button to run the applicable exposure models. If required model inputs have not been provided, a message will appear instructing the modeler to enter those values. An additional message will appear when all model runs are complete.

Model Selection INH-03 DER-01

For this scenario, emission rates, exposure concentrations, and exposure doses will be estimated using the listed model(s).

INH03: Product Sprayed
DER01: Product Applied to Skin - Absorption Fraction Method

b Run CEM Models

a Option for Inhalation Models Only

- Save final estimates only (faster)
- Save intermediate estimates (increased run time)

2. Algorithms and inputs for each model are displayed on separate subtabs for transparency and model evaluation. Each model subtab provides the relevant equations necessary to run the model, and the inputs for those equations.
 - a. Clicking on an input will populate information in the Parameter Information pane, on the right side of the page. This text provides an explanation of the clicked variable, sources of automated inputs, and relevant assumptions applied to the input.

Model Selection INH-01 DER-01a

Product Applied to a Surface Indoors Incremental Source Model (Eq 3-44)

$$ER(t) [mg/hr] = M/ta [(1 - e^{-k(t - ta)}) - (1 - e^{-k(t - ta)}) \times Ht-ta]$$

ER(t) = Emission rate at time t (mg/hr)

M = Chemical mass to be emitted (mg)

ta = Application time t (hr)

k = First-order rate constant for emissions decline (1/hr)

t = Time (hr)

H(t-ta) = 0 if t-ta < 0; 1 if t-ta > 0

Potential Lifetime Average Daily Dose (LADD) (Eq 3-49)

$$Chronic\ ADD [mg/kg-day] = C * InhR * FQcr * Duration * EDcr / BW * ATcr * CF$$

CADD = Potential Chronic Average Daily Dose (mg/kg-day)

C = Concentration (mg/m3)

InhR = Inhalation rate (m3/hr)

FQcr = Frequency of use - chronic (events/day)

Duration = Duration of use (min)

EDcr = Exposure duration - chronic (years)

BW = Body weight (kg)

ATcr = Averaging time - chronic (years)

CF = Conversion factor (365 days/year)

First-order rate constant, k (Eq 3-43)

$$k [1/hr] = \ln(10) / EvapTime$$

k [1/hr] = ln(10) / EvapTime

Evaporation time, (Eq 3-42)

$$EvapTime [hr] = 145 / (MW * VP)^{0.35540}$$

EvapTime [hr] = 145 / (MW * VP)^{0.35540}

MW = Molecular Weight (hr)

VP = Vapor Pressure (torr)

Potential Acute Dose Rate (ADR) (Eq 3-52)

$$ADR [mg/kg-day] = C * InhR * FQac * Duration * EDac / BW * ATac$$

ADR = Potential Acute Dose Rate (mg/kg-day)

C = Concentration (mg/m3)

InhR = Inhalation rate (m3/hr)

FQac = Frequency of use - acute (events/day)

Duration = Duration of use (min)

EDac = Exposure duration - acute (days)

BW = Body weight (kg)

ATac = Averaging time - acute (days)

Parameter Information ?

Description:

The duration of use is the amount of time in minutes that a product or article is used each time it is used (i.e., per use event). CEM provides default values of this input for many products/articles. Different use durations can be used for the acute and chronic exposure assessments.

Primary sources of data, methods or assumptions:

Please see the "Product Properties Sources" lookup table on the Lookup Tables and VBA Code tab for further information on parameter source information specific to each product.

4. Results tab

1. Scenario 2. Inputs 3. CEM Models 4. Results Lookup Tables

Cover Page Inhalation Ingestion Dermal Product/Article: General Purpose Cleaner - Apply to Surface

The results tab is empty until 'Run CEM Models' on the CEM Models tab is clicked.

1. The Cover Page sub-tab summarizes the exposure estimate by route and presents the total exposure for each receptor age group. The exposure attributed to inhalation of background air concentrations and incidental ingestion of background dust concentrations are also reported on this page for reference.

Cover Page Inhalation Ingestion Dermal **Product/Article:** Aerosol Spr **Chemical Name:** Pentanedioic acid, dimethyl ester

1 2

Receptor	Inhalation		Ingestion		Dermal		Total	
	Acute Dose Rate (mg/kg/d)	Chronic Average Daily Dose (mg/kg/d)	Acute Dose Rate (mg/kg/d)	Chronic Average Daily Dose (mg/kg/d)	Acute Dose Rate (mg/kg/d)	Chronic Average Daily Dose (mg/kg/d)	Acute Dose Rate (mg/kg/d)	Chronic Average Daily Dose (mg/kg/d)
Adult (≥21 years)	1.04E+01	1.42E-01			1.10E-01	2.10E-03	1.06E+01	1.44E-01
Youth (16-20 years)	3.86E+00	3.37E-02			0.00E+00	0.00E+00	3.86E+00	3.37E-02
Youth (11-15 years)	4.50E+00	3.94E-02			0.00E+00	0.00E+00	4.50E+00	3.94E-02
Child (6-10 years)	6.38E+00	5.58E-02			0.00E+00	0.00E+00	6.38E+00	5.58E-02
Small Child (3-5 years)	9.17E+00	8.02E-02			0.00E+00	0.00E+00	9.17E+00	8.02E-02
Infant (1-2 years)	1.13E+01	9.87E-02			0.00E+00	0.00E+00	1.13E+01	9.87E-02
Infant (<1 year)	1.20E+01	1.05E-01			0.00E+00	0.00E+00	1.20E+01	1.05E-01

2. The Results tab also includes subtabs for each of the exposure routes, and each subtab contains acute and chronic exposure estimates. These are labeled Acute Dose Rate (ADR) and Chronic Average Daily Dose (CADD), respectively.

Reports

1. Scenario 2. Inputs 3. CEM Models 4. Results 5. Reports

1

Choose a Report to View

- Full Scenario Report
- Cover Page
- Dermal Results
- Inhalation Results
- Ingestion Results
- Scenario Summary

View/Save Report:

Access PDF

The Reports tab allows for the viewing and exportation of various reports to Access or as PDFs. Six report options are available, including the Cover Page, Inhalation, Ingestion, and Dermal reports. These correspond to the information on the analogous results tabs. The Scenario Summary report provides a full list of input values used in the simulation. The Full Scenario report includes all information included in the Cover Page, Inhalation, Ingestion, Dermal, and Scenario Summary reports.

2. Summary of Models within CEM

The following section includes brief summaries of each model included in CEM. See Section 3 for further details on model equations and parameters.

INH01: Product Applied to a Surface Indoors Incremental Source Model

This model assumes a constant application rate over a user-specified duration of use. Each instantaneously applied segment has an emission rate that declines exponentially over time, at a rate that depends on the chemical's molecular weight and vapor pressure. There is a near-field model option that can be selected that seeks to capture the higher concentration in the breathing zone of a product user during use. Alternately, if the near-field option is not selected, Zone 1 is modeled as a homogeneous, well-mixed room. ([U.S. EPA, 2007](#))

INH02: Product Applied to a Surface Indoors Double Exponential Model

This model accounts for an initial fast release by evaporation, followed by a slow release dominated by diffusion. Only 25 percent of the applied mass is released because a substantial fraction of the mass becomes trapped in the painted substrate when it dries. Empirical studies support the assumption of 25 percent mass released and estimate a relationship between the fast rate of decline and vapor pressure, and between the slow rate of decline and molecular weight. There is a near-field model option that can be selected that seeks to capture the higher concentration in the breathing zone of a product user during use. Alternately, if the near-field option is not selected, Zone 1 is modeled as a homogeneous, well-mixed room. ([U.S. EPA, 2007](#))

INH03: Product Sprayed

This model assumes a small percentage of a product is aerosolized and therefore immediately available for uptake by inhalation. The percent of a product that is overspray is not well characterized. A recent study recommends values ranging from 1 to 6% based on a combination of modeled and empirical data ([Jayjock, 2012](#)). The remainder is assumed to contact the target surface, and to later volatilize at a rate that depends on the chemical's molecular weight and vapor pressure. The aerosolized portion is treated using a constant emission rate model. The remaining (non-aerosolized) mass is treated in the same manner as products applied to a surface, combining a constant application rate with an exponentially declining rate for each instantaneously applied segment. There is a near-field model option that can be selected that seeks to capture the higher concentration in the breathing zone of a product user during use. Alternately, if the near-field option is not selected, Zone 1 is modeled as a homogeneous, well-mixed room. ([U.S. EPA, 2007](#))

INH04: Product Added to Water

Model assumes emission at a constant rate over a duration that depends on the chemical's molecular weight and vapor pressure. If this duration is longer than the user-specified duration of use, then the chemical emissions are truncated at the end of the product-use cycle (i.e., in the case of a washing machine, the remaining chemical mass is assumed to go down the drain). The potential duration of emissions in this case is determined from the chemical's 90 percent evaporation time. ([U.S. EPA, 2007](#))

INH05: Product Placed in Environment

Model assumes emission at a constant rate over a duration that depends on its molecular weight and vapor pressure. If this duration exceeds the user specified duration of use, then the chemical emissions are truncated at the end of the product-use period, because the product is assumed to be removed from the house after the use period ([U.S. EPA, 2007](#)).

INH06: Article Placed in Environment

Model assumes emissions of semivolatile organic compound (SVOC) additives from articles and subsequent partitioning between indoor air, airborne particles, and settled dust over time. Multiple articles can be incorporated into one room over time based on the total exposed surface area of articles present within a room. Quasi-steady state concentrations are estimated over time as the ([Little et al., 2012](#)) fugacity based model was modified to account for removal mechanisms through air exchange and routine cleaning (i.e. vacuuming or dry sweeping).

ING01: Product Applied to Ground Outdoors

A shallow mixing model provides algorithms and inputs to assess a number of scenarios where products such as fertilizers are applied to soil. The populations considered in this model are those individuals who are potentially exposed during routine outdoor-work, including residential lawns, playgrounds, parks, recreation areas, schools, and golf courses. Note, the amount of product and the size of the application area can be adjusted. The model assumes ingestion of outdoor particles adhered to soil ([U.S. EPA, 2012b](#)).

ING02: Product Swallowed

Model assumes that the product is directly ingested as part of routine use and the mass is dependent on the weight fraction and use patterns associated with the product ([ACI, 2010](#)).

ING03: Article Mouthed

The mouthing methodology relies on a migration rate of the chemical of interest from the article of interest. When migration rate is known, model assumes that the amount of a chemical transferred into the saliva is dependent of the migration rate and estimates the amount transfers into the body through duration and frequency of mouthing patterns ([U.S. CPSC, 2014](#)).

ING04: Incidental Dust Ingestion (Article Model)

INH06 model assumes emissions of semivolatile organic compound (SVOC) additives from articles and subsequent partitioning between indoor air, airborne particles, and settled dust over time. ING04 calculates incidental ingestion of dust contaminated with levels of SVOCs as predicted by INH06 using the Tracer methodology ([U.S. CPSC, 2014](#)).

ING05: Ingestion after Inhalation (Article Model)

INH06 model assumes emissions of semivolatile organic compound (SVOC) additives from articles and subsequent partitioning between indoor air, airborne particles, and settled dust over time. ING05 calculates incidental ingestion of airborne particles that are inhaled and trapped in the upper airway ([U.S. CPSC, 2014](#)).

DER01: Product Applied to Skin, Fraction Absorbed Model

For products that come in direct contact with the skin, the dermal portion of the User-Defined scenario allows modeling of dermal exposure based on potential or absorbed doses. Potential dose is the amount of a chemical contained in bulk material that is applied to the skin and represents an upper bound of exposure ([U.S. EPA, 2007](#)).

DER02: Product Applied to Skin, Permeability Model

For products that come in direct contact with the skin, the dermal portion of the User-Defined scenario allows modeling of dermal exposure based on potential or absorbed doses. For products for which a skin permeability coefficient is known or if the user is interested in the amount of chemical that is, the absorbed dose methodology can be

implemented. See Section 4 for a discussion of how estimation of absorbed dose may be refined in future versions of CEM ([U.S. EPA, 2007](#)).

DER03: Article where Skin Contact Occurs

For articles that come into direct contact with the skin, the potential dermal dose is estimated by multiplying the thickness of the contact layer of the article by the density and weight fraction to estimate a loading on the surface of the article. An age-specific transfer coefficient describing the transfer of the SVOC from the surface of the article to the hands is combined with age-specific activity patterns to estimate potential loading on the skin. The amount of skin exposed will vary depending on the type of article a receptor comes into contact with ([ECETOC, 2012](#); [Delmaar et al., 2005](#)).

DER04: Direct Transfer from Vapor Phase to Skin (Article Model)

Dermal exposure can also occur from gas-phase chemical deposition directly onto the skin from the air, with subsequent absorption. The potential skin loading is calculated as the product of the gas-phase chemical concentration and the partitioning between air and skin lipids, which in turn is dependent on the octanol-air partitioning coefficient, Henry's Law coefficient (or air-water partitioning coefficient), the ideal gas law constant, and temperature ([Weschler and Nazaroff, 2012](#)).

3. Detailed Description of Models and Equations used within CEM

CEM predicts exposure via three pathways: inhalation, ingestion, and dermal. Exposure can occur via direct contact with a product or article or by contact with an exposure medium (e.g., air, dust, soil.) Exposure media concentrations, particularly air, can be dynamic in time. CEM predicts indoor air concentrations resulting from product use by implementing a deterministic, mass-balance calculation. (Indoor concentrations of air and dust from article usage in model INH06 are determined in an alternate manner and are described in section INH06.)

How a product's chemical emissions are represented in CEM depends on how the product is used and its chemical makeup. Emissions are estimated over a period of 60 days using the following equations and methods that account for how a product is used or applied, the total applied mass of the product, the weight fraction of the chemical in the product, and the molecular weight and vapor pressure of the chemical. Sections INH01 through INH05 describe the emission equations used by different product categories. Emissions from articles and associated media concentrations are estimated over a one year period in models INH01, ING04, ING05, and DER04.

Two-zone Mass Balance Model for Estimating Inhalation Exposure

CEM predicts indoor air concentrations by implementing a deterministic, mass-balance calculation. The model uses a two-zone representation of a house, school, and office building with zone 1 representing the area where the consumer product is used (e.g., a kitchen) and zone 2 being the remainder of the building of use. The modeled concentrations in the two zones are a function of the time-varying emission rate in zone 1, the volumes of zones 1 and 2, the air flows between each zone and outdoors, and the air flows between the two zones. For a conservative estimate of exposure, indoor sinks are assumed not to exist except in the case of SVOC emissions from articles (INH06). The model requires the conservation of pollutant mass as well as the conservation of air mass. CEM uses a set of differential equations whereby the time-varying concentration of the chemical in each zone is a function of the rate of pollutant loss and gain for that zone. These relationships can be expressed as shown in Figure 1 and the equations for Zone 1 and Zone 2:

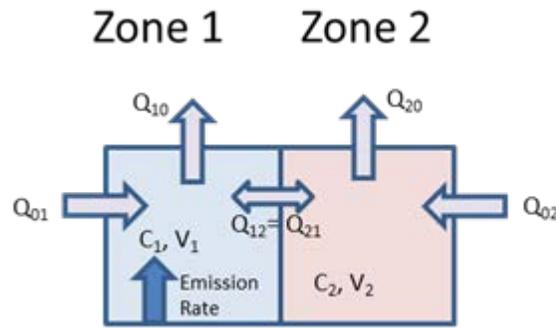


Figure 1: Schematic of two zone model of indoor environment

$$\text{Zone 1: } \frac{\partial C_1}{\partial t} = -AER_1 \times C_1 - \frac{Q_{12} \times C_1}{V_1} + \frac{E(t)}{V_1} + \frac{Q_{12} \times C_2}{V_1}$$

$$\text{Zone 2: } \frac{\partial C_2}{\partial t} = AER_2 \times C_2 + \frac{Q_{12} \times C_1}{V_2} - \frac{Q_{12} \times C_2}{V_2}$$

Where:

$\frac{\partial C}{\partial t}$ = Change in concentration with time ($\mu\text{g}/\text{m}^3/\text{hr}$)

AER = Air exchange rate in Zone 1 or 2, equivalent to Q_{0x}/V_x (hr^{-1})

C = Airborne concentration in Zone 1 or 2 ($\mu\text{g}/\text{m}^3$)

Q_{12} = Interzonal air flow (m^3/hr)

$E(t)$ = Emission rate at time, t ($\mu\text{g}/\text{hr}$)

V = Volume of Zone 1 or 2 (m^3)

The flow rates are input as constants. The pollutant mass balance is used in conjunction with the flow rates to predict the time-varying pollutant concentrations in each of the two indoor zones. The differential equations are solved using the linear solver for ordinary differential equations (LSODE) on the Python software platform.

Interzonal air flow is a variable that can be edited. The default interzonal air flows are a function of the overall air exchange rate and volume of the building, as well as the “openness” of the room itself. Kitchens, living rooms, garages, schools, and offices are considered to be more open to the rest of the home or building of use; bedrooms, bathrooms, laundry rooms, and utility rooms are usually accessed through one door and are considered more closed. The default interzonal air flow equations are based on a regression analysis by [\(U.S. EPA, 1995\)](#) and are as follows:

$$\text{Closed rooms: } Q_{12} = (0.078 + 0.31 \times AER) \times V$$

$$\text{Open rooms: } Q_{12} = (0.046 + 0.39 \times AER) \times V$$

Where:

AER = Air exchange rate of building (hr^{-1})

V = Volume of building (m^3)

Two default use environments are presented that differ from the two-zone model: Automobile and Outside. The Automobile is modeled as a one zone model with a high ($12.5 hr^{-1}$) air exchange rate. The mass of a product that is selected to be used outdoors is reduced by an empirical surrogate dilution factor of twenty. This dilution factor was calculated using [Klepeis et al. \(2009\)](#) measurements of carbon monoxide taken on a patio at a given distance and direction from a source with a known emission rate under varying wind conditions. The results at 0.25 m (the closest receptor reported) from the source were averaged and compared to the airborne concentrations modeled in a well-mixed room corresponding to the Living Room in CEM with the same emission rate and were found to be approximately a factor of 20 lower.

Near-field option for Estimating Exposure During Use

To account for scenarios which deviate from the assumption of inhalation exposure occurring in one of two well mixed zones, the CEM model offers the option of a “near-field far-field” (NFFF) model. The NFFF model accounts for imperfect mixing by conceptually dividing the room containing the emission source into two separate zones: the near-field zone, in which the product is assumed to be used and the product user’s exposure occurs, and the far-field zone, which exchanges air with the near-field zone as well as the second well mixed zone and the outdoors.

Figure 2 illustrates the assumed air exchange mechanics within the NFFF model. Chemical dispersion in the model is described by means of a system of first-order, first-degree differential equations that maintain chemical mass balance. Table 1 lists the symbols, and their corresponding definitions, used in Figure 1 and in the derivation of the governing differential equations.

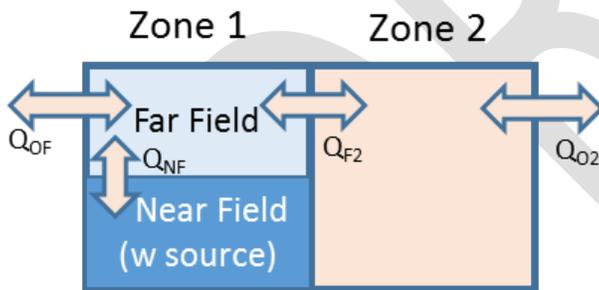


Figure 2. Air Flows in the Near-Field Far-Field Model

Table 1: Guide to Symbols Used in NFFF Model Equations

Symbol	Definition
V_{NF}	Volume of the near field in Zone 1 (m^3)
V_{FF}	Volume of the far field in Zone 1 (m^3)
V_{R2}	Volume of Zone 2 (m^3)
Q_{OF}	Ventilation rate of Zone 1 to external environment (m^3/hr)
Q_{O2}	Ventilation rate of Zone 2 to external environment (m^3/hr)
Q_{f2}	Ventilation rate between Zone 1 and Room 2 (m^3/hr)

Q_{NF}	Ventilation rate between the near field and far field (m^3/hr)
AER_{R1}	Air exchange rate of Zone 1 computed as $Q_{R1}/(V_{NF}+V_{FF})$ (/hr)
AER_{R2}	Air exchange rate of Zone 2 computed as $Q_{R2}/(V_{R2})$ (/hr)
AER_{NF}	Air exchange rate between near field and far field computed as Q_{NFFF}/V_{NF} (/hr)
t	Time (hr)

The following equations define the chemical mass exchange dynamics in the near field of Zone 1, the far field of Zone 1, and Zone 2, respectively.

Near Field, Zone 1

$$\frac{dC_{NF}}{dt} = -AER_{NF} \times C_{NF} + AER_{NF} \times C_{FF} + \frac{E(t)}{V_{NF}}$$

Far Field, Zone 1

$$\frac{dC_{FF}}{dt} = -AER_{NF} \times C_{FF} \times \frac{V_{NF}}{V_{FF}} + AER_{NF} \times C_{NF} \times \frac{V_{NF}}{V_{FF}} + Q_{R1R2} \times \frac{C_{R2}}{V_{FF}} - AER_{R1} \times C_{FF} \times \frac{(V_{NF}+V_{FF})}{V_{FF}} - Q_{R1R2} \times \frac{C_{FF}}{V_{FF}}$$

Zone 2

$$\frac{dC_{R2}}{dt} = Q_{R1R2} \times \frac{C_{FF}}{V_{R2}} - AER_{R2} \times C_{R2} - Q_{R1R2} \times \frac{C_{R2}}{V_{R2}}$$

The CEM model solves this system of equations to derive instantaneous estimates of chemical concentrations in each zone of the model, i.e. in the near field of Zone 1, the far field of Zone 1, and in Zone 2. When solving these equations, the CEM model applies a concentration ceiling corresponding to the chemical's saturation vapor pressure. The CEM model allows users to define emission rates according to five alternative emission scenarios, or according to a user-specified constant emission rate.

INH01: Product Applied to a Surface Indoors Incremental Source Model

For a product that is applied to surface, such as a general purpose cleaner or a latex paint, an incremental source model is used. This model assumes a constant application rate over the specified duration of use; each instantaneously applied segment has an emission rate that declines exponentially over time, at a rate that depends on the chemical's molecular weight (MW) and vapor pressure (VP). There is an option to model near-field exposure which determines whether to use the near-field use area directly around the product user for exposure (Use Near-Field Area in Zone 1) or a homogenous concentration for the entire room (Do Not Use Near-Field Area in Zone 1). The equation for exponentially declining emissions for each instantaneously applied segment is as follows:

$$ER(t) = ER(0) \times e^{-kt}$$

Where:

$ER(t)$ = Emission rate at time t (mg/min)

$ER(0)$ = Initial emission rate at time 0 (mg/min)

k = First-order rate constant for emissions decline (min^{-1})

t = Elapsed time (min).

The value of k is determined from an empirical relationship, developed by (Chinn, 1981), between the time required for 90% of a pure chemical film to evaporate ($EvapTime$) and the chemical's molecular weight (MW) and vapor pressure (VP):

$$EvapTime = \frac{145}{(MW \times VP)^{0.9546}}$$

The value of k is determined from the 90 percent evaporation time as follows:

$$k = \frac{\ln(10)}{EvapTime \times 60}$$

$ER(0)$ can be determined from the fact that the integral of the above $ER(t)$ equation, which accounts for all chemical mass released (i.e., *applied mass* \times *chemical weight fraction*), is equal to $ER(0) \div k$. However, the equation for the time-varying emission rate resulting from the combination of constant application and exponentially declining emissions (Evans, 1994) requires knowledge of only the total mass released and k .

$$ER(t) = \frac{M \times WF \times CF}{t_a} \times \left[(1 - e^{-k(t-t_{start})}) - ((1 - e^{-k(t-(t_{start}+t_a))}) \times H(t)) \right]$$

Where:

$ER(t)$ = Emission rate at time t (mg/min)

M = Mass of product used (g)

WF = Weight fraction of chemical in product (unitless)

CF = Conversion factor (1000 mg/g)

t_{start} = Time of start of application (min)

t_a = Application time (min)

k = First-order rate constant for emissions decline (min^{-1})

t = Time (min)

$H(t)$ = 0 if $t - (t_{start} + t_a) < 0$

= 1 if $t - (t_{start} + t_a) > 0$

The mass of product used (M) can be specified directly or estimated from the volume of product used, product density, and product dilution.

$$M = Vol \times Den \times Dil \times 10^6$$

Where:

M = Mass of product used (g)

Vol = Volume of product (m^3)

- Den* = Product density (g/cm³)
Dil = Product dilution fraction (unitless)

Because the saturation vapor pressure concentration (C_{sat}) is the highest concentration that could be present in air, CEM uses it as an upper-bound cap to estimated or user-defined zone air concentrations. The gas phase saturation concentration can be estimated with the following equation, where R = universal gas constant (8.314 J/mol-K) and T = temperature in Kelvin (298), if an experimentally derived value is not available:

$$C_{sat} = \frac{((1.33 \times 10^5) \times VP \times MW)}{(R \times T)}$$

Where:

- C_{sat} = Saturation concentration in air (ug/m³)
 VP = Vapor pressure (torr)
 MW = Molecular weight (g/mol)
 R = Universal gas constant, 8.314 J/mol-K
 T = Temperature (K)

At each time step CEM checks whether the current value for the emission rate results in an indoor concentration that exceeds the C_{sat} . If so, then the emission rate is reduced to a value that results in the indoor concentration equaling C_{sat} . In such a case, CEM keeps track of the cumulative mass that has been subtracted to meet the C_{sat} constraint. Release of this accumulated excess mass is initiated at a later point in time, when the modeled concentration otherwise would be below the C_{sat} value. This procedure is continued until all excess mass has been release, unless the model run period of 60 days ends first (or the product is removed or goes down the drain).

INH02: Product Applied to a Surface Indoors Double Exponential Model

Products with an initial fast release governed by evaporation and a later slower release dominated by diffusion have their exposure estimated via the double exponential model. Latex paint is an example. Only 25% of the applied chemical mass is released, because a substantial fraction of the mass becomes trapped in the painted substrate when it dries. Empirical studies reported by ([Wilkes et al., 1996](#)) support the assumption of 25% mass released and have estimated a relationship between the fast rate of decline (k_1) and vapor pressure (VP), and between the slow rate of decline (k_2) and molecular weight (MW), leading to the equation below for the time-varying emission rate ([Evans, 1994](#)). There is an option to model near-field exposure which determines whether to use the near-field use area directly around the product user for exposure (Use Near-Field Area in Zone 1) or a homogenous concentration for the entire room (Do Not Use Near-Field Area in Zone 1).

$$ER(t) = \frac{M \times WF \times CF}{t_a} \times \left\{ \left[f \times (1 - e^{-k_1(t-t_{start})}) + (1 - f) \times (1 - e^{-k_2(t-t_{start})}) \right] - \left[f \times (1 - e^{-k_1(t-(t_{start}+t_a))}) + (1 - f) \times (1 - e^{-k_2(t-(t_{start}+t_a))}) \right] \right\} \times H(t)$$

Where:

$ER(t)$	=	Emission rate at time t (mg/min)
M	=	Mass of product used (g)
WF	=	Weight fraction of chemical in product (unitless)
CF	=	Conversion factor (1000 mg/g)
t_{start}	=	Time of start of application (min)
t_a	=	Application time (min)
f	=	Fraction of mass emitted from first exponential (0.1) (unitless)
t	=	Time (min)
$H(t)$	=	0 if $t - (t_{start} + t_a) < 0$ 1 if $t - (t_{start} + t_a) > 0$
k_1	=	$233.25 \times (VP \div 24) \div 60$ (min ⁻¹)
k_2	=	$0.0000584 \times (MW \div 24) \div 60$ (min ⁻¹)
VP	=	Vapor pressure (torr)
MW	=	Molecular weight (g/mol)

The equation for the resultant emission profile requires estimates of the total mass released, k_1 and k_2 , and the fraction of released mass associated with the first exponential ([Evans, 1994](#)). Based on the empirical studies reported by ([Wilkes et al., 1996](#)), CEM associates 10% of the released mass with the first exponential.

The mass of product used (M) can be specified directly or estimated from the volume of product used, product density, and product dilution.

$$M = Vol \times Den \times Dil \times 10^6$$

Where:

M	=	Mass of product used (g)
Vol	=	Volume of product (m ³)
Den	=	Product density (g/cm ³)
Dil	=	Product dilution fraction (unitless)

At each time step CEM checks whether the current value for the emission rate results in an indoor concentration that exceeds the C_{sat} . If so, then the emission rate is reduced to a value that results in the indoor concentration equaling C_{sat} . See INH01 for further details.

INH03: Product Sprayed

Model assumes a small percent of product is aerosolized and therefore immediately available for uptake by inhalation. The remainder is assumed to contact the target surface, and to later volatilize at a rate that depends on the chemical's molecular weight and vapor pressure. The aerosolized portion is treated using a constant emission rate model. The

amount of mass aerosolized varies by product type and updated defaults from CONSEXPO ([Delmaar et al., 2005](#)) have been incorporated. The remaining (non-aerosolized) mass is treated in the same manner as products applied to a surface, combining a constant application rate with an exponentially declining rate for each instantaneously applied segment. There is an option to model near-field exposure which determines whether to use the near-field use area directly around the product user for exposure (Use Near-Field Area in Zone 1) or a homogenous concentration for the entire room (Do Not Use Near-Field Area in Zone 1) ([U.S. EPA, 2007](#)).

$$ER_1(t) = \frac{M \times WF \times CF \times f}{t_a} \times [1 - H(t)]$$

Where:

$ER_1(t)$ = Emission rate at time t from initial aerosolized product (mg/min)

M = Mass of product used (g)

WF = Weight fraction of chemical in product (unitless)

CF = Conversion factor (1000 mg/g)

f = Fraction aerosolized (unitless)

t_a = Application time (min)

$H(t)$ = 0 if $t - (t_{start} + t_a) < 0$

= 1 if $t - (t_{start} + t_a) > 0$

$$ER_2(t) = \frac{M \times WF \times CF}{t_a} \times \left[(1 - e^{-k(t-t_{start})}) - \left((1 - e^{-k(t-(t_{start}+t_a))}) \times H(t) \right) \right]$$

Where:

$ER_2(t)$ = Emission rate at time t from secondary surface-contacted product (mg/min)

M = Mass of product used (g)

WF = Weight fraction of chemical in product (unitless)

CF = Conversion factor (1000 mg/g)

t_{start} = Time of start of application (min)

t_a = Application time (min)

k = First-order rate constant for emissions decline (min^{-1})

t = Time (min)

$H(t)$ = 0 if $t - (t_{start} + t_a) < 0$

= 1 if $t - (t_{start} + t_a) > 0$

$$ER_{final}(t) = ER_1(t) + ER_2(t)$$

Where:

$ER_{final}(t)$ = Final emission rate at time t (mg/min)

$ER_1(t)$ = Emission rate at time t from initial aerosolized product (mg/min)

$ER_2(t)$ = Emission rate at time t from secondary surface-contacted product (mg/min)

The mass of product used (M) can be specified directly or estimated from the volume of product used, product density, and product dilution.

$$M = Vol \times Den \times Dil \times 10^6$$

Where:

M = Mass of product used (g)

Vol = Volume of product (m³)

Den = Product density (g/cm³)

Dil = Product dilution fraction (unitless)

At each time step CEM checks whether the current value for the emission rate results in an indoor concentration that exceeds the C_{sat} . If so, then the emission rate is reduced to a value that results in the indoor concentration equaling C_{sat} . See INH01 for further details.

INH04: Product Added to Water

Model assumes emission at a constant rate over a duration that depends on its molecular weight and vapor pressure. If this duration is longer than the user-specified duration of use, then the chemical emissions are truncated at the end of the product-use cycle (i.e., in the case of a washing machine, the remaining chemical mass is assumed to go down the drain). The potential duration of emissions in this case is determined from the chemical's 90 percent evaporation time.

$$EvapTime = \frac{145}{(MW \times VP)^{0.9546}} \times 60$$

Where:

$EvapTime$ = Evaporation time (min)

MW = Molecular weight (g/mol)

VP = Vapor pressure (torr)

$$ER(t) = \frac{M \times WF \times CF}{EvapTime} \times H(t)$$

Where:

$ER(t)$ = Emission rate at time t (mg/min)

M = Mass of product used (g)

WF = Weight fraction of chemical in product (unitless)

CF = Conversion factor (1000 mg/g)

$H(t)$ = 1 if $t - (t_{start} + t_{max}) < 0$

- = 0 if $t - (t_{start} + t_{max}) > 0$
- t_{start} = Time of start of application (min)
- t_a = Application time (min)
- t_{max} = Minimum between EvapTime and t_a (min)

The mass of product used (M) can be specified directly or estimated from the volume of product used, product density, and product dilution.

$$M = Vol \times Den \times Dil \times 10^6$$

Where:

- M = Mass of product used (g)
- Vol = Volume of product (m³)
- Den = Product density (g/cm³)
- Dil = Product dilution fraction (unitless)

At each time step CEM checks whether the current value for the emission rate results in an indoor concentration that exceeds the C_{sat} . If so, then the emission rate is reduced to a value that results in the indoor concentration equaling C_{sat} . See INH01 for further details.

INH05: Product Placed in Environment

Model assumes emission at a constant rate over a duration that depends on its molecular weight and vapor pressure. If this duration exceeds the user specified duration of use, then the chemical emissions are truncated at the end of the product-use period, because the product is assumed to be removed from the house after the use period ([U.S. EPA, 2007](#)).

In certain cases the source models could lead to predicted concentrations that exceed the chemical's saturation concentration in air. However, the model adjusts the time-varying emission rate so that the saturation concentration is never exceeded. In such cases, the chemical mass will be released at a slower rate than implied by the source models, once the saturation concentration is reached. The same chemical mass ultimately will be released, except in cases where emissions are truncated at the end of the product use period.

$$EvapTime = \frac{145}{(MW \times VP)^{0.9546}} \times 60$$

Where:

- $EvapTime$ = Evaporation time (min)
- MW = Molecular weight (g/mol)
- VP = Vapor pressure (torr)

$$ER(t) = \frac{M \times WF \times CF}{EvapTime} \times H(t)$$

Where:

- $ER(t)$ = Emission rate at time t (mg/min)
 M = Mass of product used (g)
 WF = Weight fraction of chemical in product (unitless)
 CF = Conversion factor (1000 mg/g)
 $H(t)$ = 0 if $t - (t_{start} + t_a) < 0$
= 1 if $t - (t_{start} + t_a) > 0$
 t_{start} = Time of start of application (min)
 t_a = Application time (min)

The mass of product used (M) can be specified directly or estimated from the volume of product used, product density, and product dilution.

$$M = Vol \times Den \times Dil \times 10^6$$

Where:

- M = Mass of product used (g)
 Vol = Volume of product (m^3)
 Den = Product density (g/cm^3)
 Dil = Product dilution fraction (unitless)

At each time step CEM checks whether the current value for the emission rate results in an indoor concentration that exceeds the C_{sat} . If so, then the emission rate is reduced to a value that results in the indoor concentration equaling C_{sat} . See INH01 for further details.

Calculation of Inhalation Dose from Product Usage

Two different inhalation dose calculations are performed in CEM: the Potential Chronic Average Daily Dose (CADD) and the Potential Acute Dose Rate (ADR). The general expression for the Potential Chronic Average Daily Dose (CADD) is as follows:

$$CADD = \frac{C_{air} \times Inh \times FQ \times Dur \times ED}{BW \times AT \times CF_1}$$

Where:

- $CADD$ = Potential Chronic Average Daily Dose (mg/kg-day)
 C_{air} = Exposure concentration (mg/m^3)
 Inh = Inhalation rate (m^3/hr)
 FQ = Frequency of product use (events/year)
 Dur = Duration of an event (hr/event)
 ED = Exposure duration (years of product usage)

- BW = Body weight (kg)
 AT = Averaging time (years)
 CF_1 = Conversion factor (365 days/year)

Within CEM, the inhalation dose is calculated iteratively, at 30 second time step intervals during the first 24 hours and every hour after that for 60 days, taking into account the chemical emission rate over time, the volume of the house and each zone, the air exchange rate and interzonal airflow rate, and the exposed individual's locations and inhalation rates during and after product use. Because of this iterative process CADD cannot be calculated directly from the LADC presented in the model results. Therefore, the CADD is calculated using the following expression:

$$CADD = \frac{Dose_{ati} \times FQ \times ED}{BW \times AT \times CF_1}$$

Where:

- $CADD$ = Potential Chronic Average Daily Dose (mg/kg-day)
 $Dose_{ati}$ = time-integrated, air dose for an event, presented in following equation (mg/event)
 FQ = Frequency of product use (events/year)
 ED = Exposure duration (years of product usage)
 BW = Body weight (kg)
 AT = Averaging time (years)
 CF_1 = Conversion factor (365 days/year)

For CADD calculations, the averaging time is one year. In turn, the time-integrated air dose is calculated as follows:

$$Dose_{ati} = \sum_{ST}^{ET} C_{i,t} \times \Delta t \times Inh_{i,t} \times CF_2$$

Where:

- $Dose_{ati}$ = time-integrated, air dose for an event (mg/event) from start time (ST) to end time (ET), where ET = ST + 60 days.
 $C_{i,t}$ = Concentration in Zone i at time t (mg/m³)
 $Inh_{i,t}$ = Inhalation Rate for Zone i at time t (m³/hr)
 Δt = time interval (1.16 x 10⁻⁴ days/event)
 CF_2 = Conversion factor (24 hours/day)

For cases where the evaporation time estimated exceeds 60 days, the model will truncate the emissions at 60 days. Conversely, for cases where the evaporation time is less than 60 days, emissions will be set to zero between the end of the evaporation time and 60 days.

The general expression for the Potential Acute Dose Rate (ADR) is as follows:

$$ADR = \frac{C_{air} \times Inh \times FQ \times Dur \times ED}{BW \times AT}$$

Where:

<i>ADR</i>	=	Potential Acute Dose Rate (mg/kg-day)
<i>C_{air}</i>	=	Exposure concentration (mg/m ³)
<i>Inh</i>	=	Inhalation rate (m ³ /hr)
<i>FQ</i>	=	Frequency of product use (events/day)
<i>Dur</i>	=	Duration of an event (hr/event)
<i>ED</i>	=	Exposure duration (days of product usage)
<i>BW</i>	=	Body weight (kg)
<i>AT</i>	=	Averaging time (days)

For the ADR calculations, an averaging time of one day is used; the ADR therefore represents the maximum time-integrated dose over a 24-hour period during the exposure event. As was the case with the CADD, ADR cannot be calculated directly. Instead, the following expression for Dose_{ati} is used:

$$Dose_{ati} = Max \left[\left[C_{i,t} \times \Delta t \times Inh_{i,t} \times CF_2 \right]_{ST}^{ET} \right]$$

Where:

<i>Dose_{ati}</i>	=	time-integrated, air dose for an event (mg/event) from start time (ST) to end time (ET), where ET = ST + 60 days.
<i>C_{i,t}</i>	=	Concentration in Zone i at time t (mg/m ³)
<i>Inh_{i,t}</i>	=	Inhalation Rate for Zone i at time t (m ³ /hr)
<i>Δt</i>	=	time interval (1.16 x 10 ⁻⁴ days/event)
<i>CF₂</i>	=	Conversion factor (24 hours/day)

For cases where the evaporation time estimated exceeds 60 days, the model will truncate the emissions at 60 days. Conversely, for cases where the evaporation time is less than 60 days, emissions will be set to zero between the end of the evaporation time and 60 days.

The exposure concentration in the above equation is calculated differently for ADR than for CADD. For the CADD calculations, CEM uses the central tendency consumer product weight fraction, duration of use, and mass of product used. In the ADR calculation, it uses the high-end consumer product weight fraction, duration of use, and mass of product used. CEM calculates all possible ADRs, over the 60-day modeling period, as running 24-hour integrations (i.e., hours 1-24, 2-25, etc.), and then reports the highest of these computed values as the ADR.

Two different inhalation concentration calculations are performed in CEM: Potential Lifetime Average Daily Concentration (LADC), and Potential Peak Concentration (Cp). They are defined as follows:

$$LADC = \frac{C_{air} \times FQ \times ED}{AT \times CF_1}$$

Where:

$LADC$ = Potential Lifetime Average Daily Concentration (mg/kg-day)

C_{air} = Exposure concentration (mg/m³)

FQ = Frequency of product use (events/year)

ED = Exposure duration (years of product usage)

AT = Averaging time (years)

CF_1 = Conversion factor (365 days/year)

The time-integrated air concentration is estimated using the following equation:

$$C_{ati} = \sum_{ST}^{ET} C_{i,t} \times \Delta t$$

Where:

C_{ati} = Time-integrated, air concentration for an event (mg/event) from start time (ST) to end time (ET), where ET = ST + 60 days.

$C_{i,t}$ = Concentration in Zone i at time t (mg/m³)

Δt = time interval (3.47 x 10⁻⁴ days/event)

For cases where the evaporation time exceeds 60 days, the model will truncate the emissions at 60 days. Conversely, for cases where the evaporation time is less than 60 days, emissions will be set to zero between the end of the evaporation time and 60 days.

The potential peak concentration (C_p) provided in the model output is defined as the highest instantaneous air concentration that is calculated by the model during any 30-second time step, and should not be interpreted as a daily maximum concentration.

$$C_p = \text{Max}[[C_{i,t}]_{ST}^{ET}]$$

Where:

C_p = Potential Peak Concentration (mg/m³), evaluated as the maximum $C_{i,t}$ from t=0 to t=ET

$C_{i,t}$ = Concentration in Zone i at time t (mg/m³)

INH06: Article Placed in Environment

The mechanisms that control SVOC behavior in an indoor environment are shown in Figure 3. These include SVOC emissions, mixing within the gas phase, transfer to particulates by partitioning, removal due to ventilation, removal due

to cleaning of settled particulates and dust to which the SVOC has partitioned, and sorption or desorption to/from interior surfaces.

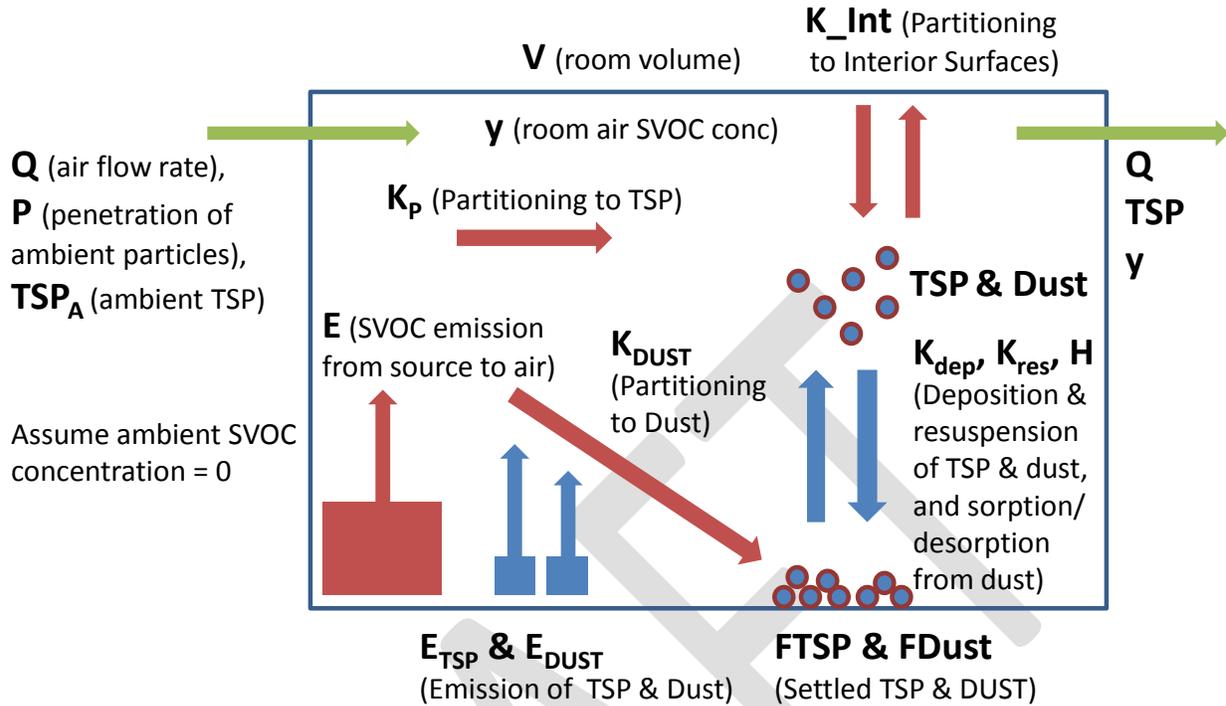


Figure 3. Schematic of fate and transport of SVOC in indoor environment

Model Description

The model provides time-varying estimates of indoor gas-phase, suspended particulate, and settled particulate SVOC concentrations based on SVOC emissions from an article located in a hypothetical indoor environment. The main features of the model include:

- SVOC emissions from the article are estimated based on a first order source decay methodology described in (ASTM, 2010).
- The model comprises an air compartment (including gas phase and suspended particulates) and a floor compartment (containing settled particulates)
- A bimodal distribution is used to account for variable particle sizes in indoor environments: coarse particulates ($>10 \mu\text{m}$ - $100 \mu\text{m}$ in diameter, referred to as “dust”); and fine particulates ($10 \mu\text{m}$ in diameter or smaller, referred to as “TSP”).
- Particulates may exist in the suspended phase in the air compartment or in the settled phase within the floor compartment of the model.
- The two distinct forms of particulates are assumed to have differential partitioning behavior with respect to air.
- Particulates, both in the suspended and settled phases, are not assumed to be in equilibrium with the air phase; chemical transfer between particulates and the air phase is kinetically modeled in terms of two-phase mass transfer theory.
- The interface area between particulate and air available for mass transfer is calculated assuming absence of agglomeration and assuming that 100% of the area is available for suspended particulates while only 50% is available for settled particulates.

- Particulate settling and resuspension processes, which act as a means for chemical mass transfer between the floor and air compartments, are incorporated into the model.
- The model tracks both the chemical inventory of SVOC in all phases of the room as well as the physical inventory of particulates in both compartments.
- The effect of periodic room cleaning, which allows depletion of the settled particulate inventory and its associated SVOC burden, is accounted for.
- The model accounts for sorption (and potentially desorption) of gas phase SVOC to other indoor surfaces (sinks) using the two-phase mass transfer methodology.

The approach summarized above effectively advances the ([Little et al., 2012](#)) screening approach to a fully mass-balanced model.

Exposure to SVOCs will occur via inhalation of both gas-phase and particle-bound SVOCs within the inhalable size range (defined as <10 μm), as well as incidental ingestion of SVOCs partitioned to settled dust. As such, while the model treats these entities separately based on mechanistic behavior, the values are combined as appropriate to estimate exposure as described in Appendix A. SVOC exposure can also occur via direct contact with articles, either by direct mouthing or dermal contact. The contribution of these exposure pathways to total exposure is captured in other models within CEM.

Calculations of exposure dose from chronic exposure to SVOC emissions from articles require slightly different assumptions than when calculating exposure due from acute exposure from products. These considerations are put forth in Appendix A.

Model Parameters

Table 1 itemizes the chemical and physical parameters and their representational symbols that feature in the set of 10-differential equations that define the model.

Table 1: Physical-Chemical Parameters Referenced in Model Equations

Symbol	Property	Units
Physical Parameters		
V	Volume of the room	m^3
Q	Ventilation rate of the room	m^3/hr
A_s	Area of emitting article surface	m^2
CT	Thickness of emitting article surface ^a	m
k_{dep}TSP	TSP deposition rate constant	hr^{-1}
k_{dep}Dust	Dust deposition rate constant	hr^{-1}
k_{res}TSP	TSP resuspension rate constant	hr^{-1}
k_{res}Dust	Dust resuspension rate constant	hr^{-1}
E_ATSP	Emission rate of TSP into indoor air	mg/hr
E_ADust	Emission rate of dust into indoor air	mg/hr
E_FTSP	Emission rate of TSP onto indoor floor	mg/hr
E_FDust	Emission rate of dust onto indoor floor	mg/hr
AmbTSPConc	Concentration of TSP in ambient air	mg/m^3
FilterPen	Air Filter Penetration Ratio	None
C_{eff}	Cleaning Efficiency	None
k_{cl}(t)	Binary switch representing whether cleaning is ongoing (based on cleaning periodicity)	None
Z(t)	Binary switch representing whether product is present in room	None
ρ_{TSP}	Density of TSP particle	mg/m^3
ρ_{Dust}	Density of dust particle	mg/m^3
r_{TSP}	Radius of TSP particle	m
r_{Dust}	Radius of dust particle	m

Symbol	Property	Units
A_{Int}	Area of interior surfaces	m^2
L_{Int}	Length of sorbing portion of interior surfaces	m
T	Point in time at which equations are being estimated	hr
Chemical Parameters		
H	SVOC gas phase mass transfer coefficient	m/hr
K_{TSP}	SVOC TSP-air partition coefficient	m^3/mg
K_{Dust}	SVOC dust-air partition coefficient	m^3/mg
K_{Art}	SVOC article-air partition coefficient	None
K_{Int}	SVOC -air partition coefficient	None
H_{TSP}	TSP overall mass transfer coefficient	m/hr
H_{Dust}	Dust overall mass transfer coefficient	m/hr
H_{Int}	Interior surfaces overall mass transfer coefficient	m/hr
C_{OArt}	Initial concentration of SVOC in emitting article	$\mu g/m^3$
Inventory Terms		
N_{air}	SVOC mass in the gas phase in	μg
N_{ATSP}	SVOC mass sorbed to suspended TSP in the air	μg
N_{ADust}	SVOC mass sorbed to suspended dust in the air	μg
N_{FTSP}	SVOC mass sorbed to settled TSP on the floor	μg
N_{FDust}	SVOC mass sorbed to settled dust on the floor	μg
N_{Int}	SVOC mass sorbed to interior surfaces	μg
A_{TSP}	Mass of TSP suspended in the floor	mg
A_{Dust}	Mass of dust suspended in the floor	mg
F_{TSP}	Mass of TSP settled on the floor	mg
F_{Dust}	Mass of dust settled on the floor	mg

^aThe thickness of emitting article surface value can impact emissions. EPA is considering article-specific thicknesses.

$$A_{int} = 2.08 \times V$$

A_{Int} = Area of Interior Surfaces

V= Volume of Room

Model Equations

The following set of 10 differential equations mathematically describe the model discussed above. Each equation has an indicative title describing the entity for which a mass balance is being carried out. When these 10 equations are solved simultaneously, the model is able to produce time-varying estimates of SVOC mass in various media as well as dust and TSP mass in air and on the floor.

Equation 1: Mass Balance for SVOC in Gas Phase

$$\begin{aligned}
 \frac{dN_{air}}{dt} = & Z(t) \times h \times A_s \times \frac{C_{0Art}}{K_{art}} \times e^{-\left(\frac{h}{K_{art} \times L_{art}} \times t\right)} \\
 & - \frac{Q}{V} \times N_{air} \\
 & - H_{TSP} \times \frac{A_{TSP}}{\rho_{TSP}} \times \frac{3}{r_{TSP}} \times \left(\frac{N_{air}}{V} - \frac{N_{ATSP}}{A_{TSP}} \times \frac{1.0}{K_{TSP}} \right) \\
 & - H_{Dust} \times \frac{A_{Dust}}{\rho_{Dust}} \times \frac{3}{r_{Dust}} \times \left(\frac{N_{air}}{V} - \frac{N_{ADust}}{A_{Dust}} \times \frac{1.0}{K_{Dust}} \right) \\
 & - H_{TSP} \times \frac{F_{TSP}}{\rho_{TSP}} \times \frac{1.5}{r_{TSP}} \times \left(\frac{N_{air}}{V} - \frac{N_{FTSP}}{F_{TSP}} \times \frac{1.0}{K_{TSP}} \right) \\
 & - H_{Dust} \times \frac{F_{Dust}}{\rho_{Dust}} \times \frac{1.5}{r_{Dust}} \times \left(\frac{N_{air}}{V} - \frac{N_{FDust}}{F_{Dust}} \times \frac{1.0}{K_{Dust}} \right) \\
 & - H_{Int} \times \left(\frac{N_{air}}{V} - \frac{N_{Int}}{A_{Int} \times L_{Int}} \times \frac{1.0}{K_{Int}} \right) \times A_{Int}
 \end{aligned}$$

Equation 2: Mass Balance for SVOC Sorbed to Suspended TSP

$$\begin{aligned}
 \frac{dN_{ATSP}}{dt} = & H_{TSP} \times \frac{A_{TSP}}{\rho_{TSP}} \times \frac{3}{r_{TSP}} \times \left(\frac{N_{air}}{V} - \frac{N_{ATSP}}{A_{TSP}} \times \frac{1.0}{K_{TSP}} \right) \\
 & + kres_{TSP} \times N_{FTSP} - kdep_{TSP} \times N_{ATSP} - \frac{Q}{V} \times N_{ATSP}
 \end{aligned}$$

Equation 3: Mass Balance for SVOC Sorbed to Suspended Dust

$$\begin{aligned}
 \frac{dN_{ADust}}{dt} = & H_{Dust} \times \frac{A_{Dust}}{\rho_{Dust}} \times \frac{3}{r_{Dust}} \times \left(\frac{N_{air}}{V} - \frac{N_{ADust}}{A_{Dust}} \times \frac{1.0}{K_{Dust}} \right) \\
 & + kres_{Dust} \times N_{FDust} - kdep_{Dust} \times N_{ADust} - \frac{Q}{V} \times N_{ADust}
 \end{aligned}$$

Equation 4: Mass Balance for SVOC Sorbed to Settled TSP

$$\begin{aligned}
 \frac{dN_{FTSP}}{dt} = & H_{TSP} \times \frac{F_{TSP}}{\rho_{TSP}} \times \frac{1.5}{r_{TSP}} \times \left(\frac{N_{air}}{V} - \frac{N_{FTSP}}{F_{TSP}} \times \frac{1.0}{K_{TSP}} \right) \\
 & - kres_{TSP} \times N_{FTSP} + kdep_{TSP} \times N_{ATSP} - k_{cl}(t) \times Cl_{eff} \times N_{FTSP}
 \end{aligned}$$

Equation 5: Mass Balance for SVOC Sorbed to Settled Dust

$$\frac{dN_{FDust}}{dt} = H_{Dust} \times \frac{F_{Dust}}{\rho_{Dust}} \times \frac{1.5}{r_{Dust}} \times \left(\frac{N_{air}}{V} - \frac{N_{FDust}}{F_{Dust}} \times \frac{1.0}{K_{Dust}} \right) - kres_{Dust} \times N_{FDust} + kdep_{Dust} \times N_{ADust} - k_{cl}(t) \times Cl_{eff} \times N_{FTSP}$$

Equation 6: Mass Balance for SVOC Sorbed to Interior Surfaces (Sinks)

$$\frac{dN_{int}}{dt} = H_{Int} \times \left(\frac{N_{air}}{V} - \frac{N_{Int}}{A_{Int} \times L_{Int}} \times \frac{1.0}{K_{Int}} \right) \times A_{Int}$$

Equation 7: Mass Balance for Suspended TSP

$$\frac{dA_{TSP}}{dt} = E_{ATSP} + Q \times AmbTSPConc \times FilterPen - \frac{Q}{V} \times A_{TSP} - kdep_{TSP} \times A_{TSP} + kres_{TSP} \times F_{TSP}$$

Equation 8: Mass Balance for Suspended Dust

$$\frac{dA_{Dust}}{dt} = E_{ADust} - \frac{Q}{V} \times A_{Dust} - kdep_{Dust} \times A_{Dust} + kres_{Dust} \times F_{TSP}$$

Equation 9: Mass Balance for Settled TSP

$$\frac{dF_{TSP}}{dt} = E_{FTSP} + kdep_{TSP} \times A_{TSP} - kres_{TSP} \times F_{TSP} - k_{cl}(t) \times Cl_{eff} \times F_{TSP}$$

Equation 10: Mass Balance for Settled Dust

$$\frac{dF_{dust}}{dt} = E_{FDust} + kdep_{Dust} \times A_{Dust} - kres_{Dust} \times F_{Dust} - k_{cl}(t) \times Cl_{eff} \times F_{Dust}$$

Estimation of Chemical Parameters from Basic Physical-Chemical Properties

As noted in Table 1, the model depends on a number of chemical parameters that users have the freedom to specify. In situations where users may not have access to sources of values for those parameters, the model can deploy “default” equations that depend on basic physical and chemical properties to estimate the required parameters. This section describes the default estimating equations.

Estimating the gas phase mass transfer coefficient

The gas phase mass transfer coefficient can be estimated using the relationships applied in the AMEM model. These include mass transfer from vertical surfaces, mass transfer from horizontal surfaces, and mass transfer dominated by thermal convection. While the authors consider each case, they conclude that mass transfer in indoor environments is dominated by thermal convection. Equations 4-35 and 4-21 from the AMEM guidance ([U.S. EPA, 2007](#)) are combined, along with constants necessary to convert from cm/s to m/hr (1m/100cm and 3600s/hr), to result in the following estimation for mass transfer:

$$h = 46.8 \times \frac{3.3}{(2.5+MW^{1/3})^2} \quad (11)$$

Where:

h = gas phase mass transfer coefficient for SVOC between bulk air and surface (m/hr)

MW = molecular weight (g/mol)

The AMEM methodology for estimating the mass transfer coefficient was incorporated. PARAMS is another EPA model that can estimate the mass transfer coefficient. The methodology presented here is believed to be applicable to foams as well as solid polymers. While foams have the potential for higher convection rates than solid polymers, [Little et al. \(2012\)](#) demonstrates in the supporting information that this value is negligible compared to diffusive emissions from the nominal surface area of the foam.

Estimating K_{TSP} and K_{Dust}

The particle-air partitioning coefficient (K_p , expressed in units of mg/m^3) can be estimated using the following general equation, where 'part' refers to either TSP or Dust as appropriate ([Little et al., 2012](#)):

$$K_p = f_{om_part} \times \frac{K_{oa}}{\rho_{part}} \quad (12)$$

Where:

K_p = SVOC partition coefficient for TSP (K_{TSP}) or dust (K_{Dust}) (m^3/mg)

f_{om_part} = volume fraction organic matter in airborne particles; suggested value 0.4 (unitless)

K_{oa} = partitioning coefficient between octanol and air (unitless)

ρ_{part} = density of airborne particles; suggested value 1×10^9 (mg/m^3)

The particle-air and dust-air partitioning coefficients can also be estimated using the vapor pressure. However, this methodology is specific to each additive-solid combination and relies on experimentally determined empirical constants that are available for a limited number of combinations. This methodology for estimating partitioning is available in PARAMS ([U.S. EPA, 2005](#)) and we recommend using PARAMS if additional partitioning estimates are required.

Estimating K_{art} and K_{int}

Solid-air SVOC partition coefficients, such as K_{art} and K_{int} , are used to describe partitioning from the source to the air (art) and from air to an indoor sink (int). These parameters may be estimated based on SVOC vapor pressure using the following relationship, where 'solid' refers to either Art or Int as appropriate ([U.S. EPA, 2005](#)):

$$\ln(K_{solid}) = 8.86 - 0.785 \times \ln(V_p) \quad (13)$$

Where:

K_{solid} = the solid-air SVOC partition coefficient (dimensionless)

V_p = the vapor pressure of the SVOC (mm Hg)

Estimating H_{Int} , H_{Dust} and H_{TSP}

$$D_s = \frac{0.000000000003}{(MW \div 292)^{0.65}}$$

Where:

D_s = Solid-phase diffusion coefficient (m^2/hr)

MW = Molecular weight (g/mol)

$$K_{solid} = e^{(8.86 - 0.785 \times \ln(VP))}$$

Where:

K_{solid} = Solid-air partition coefficient (unitless)

VP = Vapor pressure (torr)

$$h_a = 46.8 \times (3.3 \div (2.5 + MW^{\frac{1}{3}}))^2$$

Where:

h_a = SVOC gas phase mass transfer coefficient (m/hr)

MW = Molecular weight (g/mol)

The overall gas phase SVOC mass transfer coefficient between solid phases (such as interior surfaces, dust particles and TSP) and the air can be estimated based on the following relationship, where 'solid' refers to Int, TSP, or Dust as appropriate ([U.S. EPA, 2005](#)):

$$\frac{1}{H_{solid}} = \frac{1}{h_a} + \frac{1}{\frac{2D_s}{L}K_{solid}} \quad (14)$$

Where:

H_{solid} = Overall mass transfer coefficient for interior surface (H_{int}), TSP (H_{TSP}), or dust (H_{Dust}) (m/hr)

h_a = the SVOC gas phase mass transfer coefficient (m/hr), which is estimated earlier in equation (12)

D_s = the SVOC solid-phase diffusion coefficient (m²/hr)

L = the thickness of the solid layer (m)

K_{solid} = the SVOC solid-air partition coefficient (unitless)

Estimating D

The solid phase diffusion coefficient for the SVOC may be computed based on a reference compound ([U.S. EPA, 2005](#)), as follows:

$$\left(\frac{D_0}{D_1}\right) = \left(\frac{MW_1}{MW_0}\right)^{0.65} \quad (15)$$

Where:

D_0 = 3×10^{-11} (m²/h) is the diffusion coefficient for the reference compound (PCB-52)

D_1 = diffusion coefficient for compound of interest (m²/h)

MW_0 = 292 (g/mol) is the molecular weight for the reference compound

MW_1 = molecule weight for compound of interest (g/mol)

The thickness of the solid layer may be assumed to be 0.005m for interior surfaces and equal to the radius of the particle for particulates ([Little et al., 2012](#); [ASTM, 2010](#); [U.S. EPA, 2005](#)).

The diffusion coefficient can also be estimated using the molar volume of the SVOC. However, this methodology is specific to the molecular structure of each SVOC additive. This methodology for estimating diffusion is available in PARAMS ([U.S. EPA, 2005](#)) and we recommend using PARAMS if additional partitioning estimates are required.

Note, measured values are preferred over estimated values as inputs for use of this model. A select set of measured diffusion and partitioning coefficients are presented in Tables B-12 and B-13. EPA is also considering supplementing available measured values with a small number of estimated values for parameters above from the AMEM and PARAMS models.

Calculation of Inhalation Dose from Article Exposure

Similar to inhalation exposure associated with product usage, two different inhalation dose calculations are performed in CEM: the Potential Chronic Average Daily Dose (CADD) and the Potential Acute Dose Rate (ADR). Both gas-phase and airborne TSP-bound SVOCs are assumed to be available for inhalation. The general expression for the Potential Chronic Average Daily Dose (CADD) is as follows:

$$CADD_{Air} = \frac{C_{gas_avg} \times FracTime \times InhalAfter \times CF_1}{BW \times CF_2}$$

$$CADD_{Particulate} = \frac{SVOCTSP_{air_avg} \times TSP_{air_avg} \times FracTime \times InhalAfter \times CF_1}{BW \times CF_2}$$

$$CADD_{total} = CADD_{Air} + CADD_{Particulate}$$

Where:

$CADD_{Air}$	= Potential Chronic Average Daily Dose, air (mg/kg-day)
$CADD_{Particulate}$	= Potential Chronic Average Daily Dose, particulate (mg/kg-day)
$CADD_{total}$	= Potential Chronic Average Daily Dose, total (mg/kg-day)
C_{gas_avg}	= Average gas phase concentration ($\mu\text{g}/\text{m}^3$)
$SVOCTSP_{air_avg}$	= Average SVOC in TSP concentration, air ($\mu\text{g}/\text{mg}$)
TSP_{air_avg}	= Average TSP concentration, air (mg/m^3)
$FracTime$	= Fraction of time in environment (unitless)
$InhalAfter$	= Inhalation rate after use (m^3/hr)
CF_1	= Conversion factor (24 hrs/day)
BW	= Body weight (kg)
CF_2	= Conversion factor (1000 $\mu\text{g}/\text{mg}$)

The general expression for the Potential Acute Dose Rate (ADR) is as follows:

$$ADR_{Air} = \frac{C_{gas_max} \times FracTime \times InhalAfter \times CF_1}{BW \times CF_2}$$

$$ADR_{Particulate} = \frac{SVOCTSP_{air_max} \times TSP_{air_avg} \times FracTime \times InhalAfter \times CF_1}{BW \times CF_2}$$

$$ADR_{total} = ADR_{Air} + ADR_{Particulate}$$

Where:

ADR_{Air}	= Potential Acute Dose Rate, air (mg/kg-day)
$ADR_{Particulate}$	= Potential Acute Dose Rate, particulate (mg/kg-day)
ADR_{total}	= Potential Acute Dose Rate, total (mg/kg-day)
C_{gas_max}	= Maximum gas phase concentration (ug/m ³)
$SVOCTSP_{air_max}$	= Maximum SVOC in TSP concentration, air (μg/mg)
TSP_{air_max}	= Maximum TSP concentration, air (mg/m ³)
$FracTime$	= Fraction of time in environment (unitless)
$InhalAfter$	= Inhalation rate after use (m ³ /hr)
CF_1	= Conversion factor (24 hrs/day)
BW	= Body weight (kg)
CF_2	= Conversion factor (1000 μg/mg)

ING01: Product Applied to Ground Outdoors

Model assumes ingestion of chemical mixed with soil particles after the product, such as fertilizer, is applied directly to the ground. The model divides the mass of chemical (mass of product multiplied by weight fraction of chemical) by the volume of soil (area of application multiplied by the soil mixing depth, density, and porosity) to get the concentration in the soil. Chemical decay and physical transport away from the surface soil, as well as repeat applications are accounted for in the frequency and soil half-life terms. This is multiplied by the soil ingestion rate, exposure duration, averaging time, and body weight to calculate dose ([U.S. EPA, 2012b](#)).

$$CADD = \frac{M \times WF \times Freq \times 0.5^{\left(\frac{365}{t_{1/2}}\right)} \times CF_1 \times SoilIng \times CF_2 \times ED_{cr}}{Area \times Depth \times \rho \times (1 - \emptyset) \times AT_{cr} \times BW}$$

Where:

$CADD$	= Potential Chronic Average Daily Dose (mg/kg-day)
M	= Mass of product applied (g/use)
WF	= Weight fraction of chemical in product (unitless)
$Freq$	= Frequency of use/application (use/year)
$t_{1/2}$	= Chemical half-life in soil (days)

CF_1	=	Conversion factor (1000 mg/g)
$SoilIng$	=	Incidental soil ingestion rate (mg/day)
CF_2	=	Conversion factor (1kg/1000g)
ED_{cr}	=	Exposure duration, chronic (years)
$Area$	=	Area of yard product is applied (m ²)
$Depth$	=	Mixing depth of soil (m)
ρ	=	Soil density (kg/m ³)
\emptyset	=	Soil porosity (unitless)
AT_{cr}	=	Averaging time, chronic (years)
BW	=	Body weight (kg)

$$ADR = \frac{M \times WF \times CF_1 \times SoilIng \times CF_2 \times ED_{ac}}{Area \times Depth \times \rho \times (1 - \emptyset) \times AT_{ac} \times BW}$$

Where:

ADR	=	Potential Acute Dose Rate (mg/kg-day)
M	=	Mass of product ingested (g)
WF	=	Weight fraction of chemical in product (unitless)
CF_1	=	Conversion factor (1000 mg/g)
$SoilIng$	=	Incidental soil ingestion rate (mg/day)
CF_2	=	Conversion factor (1kg/1000g)
ED_{ac}	=	Exposure duration, acute (days)
$Area$	=	Area of yard product is applied (m ²)
$Depth$	=	Mixing depth of soil (m)
ρ	=	Soil density (kg/m ³)
\emptyset	=	Soil porosity (unitless)
AT_{ac}	=	Averaging time, acute (days)
BW	=	Body weight (kg)

ING02: Product Ingested via Swallowing

Model assumes that the product is directly ingested as part of routine use and the mass is dependent on the weight fraction and use patterns associated with the product ([ACI, 2010](#)).

$$CADD = \frac{FQ_{cr} \times M \times WF \times F_{ing} \times CF_1 \times ED_{cr}}{BW \times AT_{cr} \times CF_2}$$

Where:

$CADD$	=	Potential Chronic Average Daily Dose (mg/kg-day)
--------	---	--

FQ_{cr}	=	Frequency of use, chronic (events/year)
M	=	Mass of product used (g)
WF	=	Weight fraction of chemical in product (unitless)
F_{ing}	=	Fraction of product ingested (unitless)
ED_{cr}	=	Exposure duration, chronic (years)
AT_{cr}	=	Averaging time, chronic (years)
BW	=	Body weight (kg)
CF_1	=	Conversion factor (1000 mg/g)
CF_2	=	Conversion factor (365 days/year)

$$ADR = \frac{FQ_{ac} \times M \times WF \times F_{ing} \times CF_1 \times ED_{ac}}{BW \times AT_{ac}}$$

Where:

ADR	=	Potential Acute Dose Rate (mg/kg-day)
FQ_{ac}	=	Frequency of use, acute (events/day)
M	=	Mass of product used (g)
WF	=	Weight fraction of chemical in product (unitless)
F_{ing}	=	Fraction of product ingested (unitless)
ED_{ac}	=	Exposure duration, acute (days)
AT_{ac}	=	Averaging time, acute (days)
BW	=	Body weight (kg)
CF_1	=	Conversion factor (1000 mg/g)

ING03: Article Ingested via Mouthing (Migration Rate Method)

Model assumes that a fraction of the chemical present in the article is ingested via object to mouth contact, or mouthing where the chemical of interest migrates from the article to the saliva. When the migration rate is known, model assumes that the amount of a chemical transferred into the saliva is dependent of the migration rate and estimates the amount transfers into the body through duration and frequency of mouthing patterns ([U.S. CPSC, 2014](#)).

$$CADD = \frac{MR \times CA \times FQ \times Dur \times ED_{cr}}{BW \times AT_{cr}}$$

Where:

$CADD$	=	Potential Chronic Average Daily Dose (mg/kg-day)
MR	=	Migration rate of chemical from article to saliva (mg/cm ² /hr)

CA = Contact area of mouthing (cm²)
FQ = Frequency of mouthing (events/day)
Dur = Duration of mouthing (hrs/events)

ED_{cr} = Exposure duration, chronic (years)
AT_{cr} = Averaging time, chronic (years)
BW = Body weight (kg)

$$ADR = \frac{MR \times CA \times FQ \times Dur \times ED_{ac}}{BW \times AT_{ac}}$$

Where:

ADR = Potential Acute Dose Rate (mg/kg-day)
MR = Migration rate of chemical from article to saliva (mg/cm²/hr)
CA = Contact area of mouthing (cm²)
FQ = Frequency of mouthing (events/day)
Dur = Duration of mouthing (hrs/events)
ED_{ac} = Exposure duration, acute (days)
AT_{ac} = Averaging time, acute (days)
BW = Body weight (kg)

ING04: Incidental Dust Ingestion (Article Model)

The Article Model described in INH06 calculates SVOC concentration in small particles (termed TSP) and large particles (termed Dust) that are settled on the floor. The model assumes these particle-bound SVOCs are available via incidental dust ingestion assuming a daily dust ingestion rate and a fraction of the day that is spent in the zone with the SVOC-containing dust.

$$CADD = \frac{(SVOCTSP_{floor_avg} + SVOCDust_{floor_avg}) \times FracTime \times DustIng}{BW \times CF}$$

Where:

CADD = Potential Chronic Average Daily Dose (mg/kg-day)
SVOCTSP_{floor_avg} = Average SVOC in TSP concentration, floor (ug/mg)
SVOCDust_{floor_avg} = Average SVOC in dust concentration, floor (ug/mg)
FracTime = Fraction of time in environment (unitless)
DustIng = Dust ingestion rate (mg/day)

BW = Body weight (kg)
CF = Conversion factor (1000 ug/mg)

$$ADR = \frac{(SVOCTSP_{floor_max} + SVOCDust_{floor_max}) \times FracTime \times DustIng}{BW \times CF}$$

Where:

ADR = Potential Acute Dose Rate (mg/kg-day)
SVOCTSP_{floor_avg} = Maximum SVOC in TSP concentration, floor (ug/mg)
SVOCDust_{floor_avg} = Maximum SVOC in dust concentration, floor (ug/mg)
FracTime = Fraction of time in environment (unitless)
DustIng = Dust ingestion rate (mg/day)
BW = Body weight (kg)
CF = Conversion factor (1000 ug/mg)

The above equations assume the SVOCs are volatilized from the SVOC-containing article to the air and then partition to dust. Alternately, SVOC can partition directly from the article to dust in direct contact with the article. This is also estimated in ING04 model assuming the original SVOC concentration in the article is known, and the density of the dust and dust-air and solid-air partitioning coefficients are either known or estimated as presented in INH06. The model assumes partitioning behavior dominates, or instantaneous equilibrium is achieved. This is presented as a worst-case or upper bound scenario.

$$C_d = \frac{C_{0_art} \times K_{dust} \times \rho_{dust}}{K_{solid}}$$

Where:

C_d = Concentration of SVOC in dust (mg/cm³)
C_{0_art} = Initial SVOC concentration in article (mg/cm³)
K_{dust} = SVOC dust-air partition coefficient (m³/mg)
ρ_{dust} = Dust density (mg/m³)
K_{solid} = Solid air partition coefficient (unitless)

Once the SVOC concentration in the dust is estimated, chronic and acute dose rates can be calculated.

$$CADD_{DTD} = \frac{C_d \times FracTime \times DustIng \times CF}{\rho_{dust} \times BW}$$

Where:

- $CADD_{DTD}$ = Potential Chronic Average Daily Dose from direct transfer to dust (mg/kg-day)
 $FracTime$ = Fraction of time in environment (unitless)
 $DustIng$ = Dust ingestion rate (mg/day)
 CF = Conversion factor ($10^6 \text{ cm}^3/\text{m}^3$)
 ρ_{dust} = Dust density (mg/m³)
 BW = Body weight (kg)

$$ADR_{DTD} = \frac{C_d \times FracTime \times DustIng \times CF}{\rho_{dust} \times BW}$$

Where:

- ADR_{DTD} = Potential Acute Dose Rate from direct transfer to dust (mg/kg-day)
 $FracTime$ = Fraction of time in environment (unitless)
 $DustIng$ = Dust ingestion rate (mg/day)
 CF = Conversion factor ($10^6 \text{ cm}^3/\text{m}^3$)
 ρ_{dust} = Dust density (mg/m³)
 BW = Body weight (kg)

ING05: Ingestion after Inhalation (Article Model)

The Article Model described in INH06 estimates SVOC concentrations in small and large airborne particles. While these particles are expected to be inhaled, not all will be able to penetrate to the lungs, but will be trapped in the upper airway and subsequently swallowed. The model estimates the mass of SVOC bound to airborne small particles (TSP) and large particles (Dust) that will be inhaled and trapped in the upper airway. This fraction that is trapped in the airway is termed the ingestion fraction (IF). The mass trapped is assumed to be available for ingestion.

$$CADD_{IAI} = \frac{(SVOCTSP_{air_avg} \times TSP_{air_avg} \times IF_{TSP} + SVOCDust_{air_avg} \times Dust_{air_avg} \times IF_{Dust}) \times InhalAfter \times CF_1}{BW \times CF_2}$$

Where:

- $CADD_{IAI}$ = Potential Chronic Average Daily Dose from ingestion after inhalation (mg/kg-day)
 $SVOCTSP_{air_avg}$ = Average SVOC in TSP concentration, air (ug/mg)
 TSP_{air_avg} = Average TSP concentration, air (mg/m³)
 IF_{TSP} = TSP ingestion fraction (unitless)
 $SVOCDust_{air_avg}$ = Average SVOC dust concentration, air (ug/mg)

- $Dust_{air_avg}$ = Average dust concentration, air (mg/m³)
- IF_{Dust} = Dust ingestion fraction (unitless)
- $InhalAfter$ = Inhalation rate after use (m³/hr)
- CF_1 = Conversion factor (24 hrs/day)
- BW = Body weight (kg)
- CF_2 = Conversion factor (1000 mg/g)

$$ADR_{IAI} = \frac{(SVOCTSP_{air_max} \times TSP_{air_max} \times IF_{TSP} + SVOCDust_{air_max} \times Dust_{air_max} \times IF_{Dust}) \times InhalAfter \times CF_1}{BW \times CF_2}$$

Where:

- ADR_{IAI} = Potential Acute Dose Rate from Ingestion and Inhalation (mg/kg-day)
- $SVOCTSP_{air_max}$ = Maximum SVOC in TSP concentration, air (ug/mg)
- TSP_{air_max} = Maximum TSP concentration, air (mg/m³)
- IF_{TSP} = TSP ingestion fraction (unitless)
- $SVOCDust_{air_max}$ = Maximum SVOC in dust concentration, air (ug/mg)
- $Dust_{air_max}$ = Maximum dust concentration, air (mg/m³)
- IF_{Dust} = Dust ingestion fraction (unitless)
- $InhalAfter$ = Inhalation rate after use (m³/hr)
- CF_1 = Conversion factor (24 hrs/day)
- BW = Body weight (kg)
- CF_2 = Conversion factor (1000 mg/g)

DER01: Product Applied to Skin (Fraction Absorbed Method)

For products that come in direct contact with the skin, the dermal portion of the User-Defined scenario allows modeling dermal exposure based on potential or absorbed doses. Potential dose is the amount of a chemical contained in bulk material that is applied to the skin. ([U.S. EPA, 2007](#)). Absorbed dose is the amount of substance penetrating across the absorption barriers of an organism. The absorbed dose can be calculated by multiplying the potential dose by the user-specified fraction absorbed.

The amount of product that is retained on the skin (grams of product per square centimeter of skin surface per event or g/cm²-event) is the product of the film thickness of the liquid on the skin's surface, the density of the formulation, and the percent retained on skin (1 is assumed for potential dose, and smaller fractions can be assumed for absorbed dose).

$$AR = FT \times D \times \frac{Ret}{100}$$

AR = Amount retained on the skin (g/cm^2)

FT = Film Thickness (cm)

Den = Density of formulation (g/cm^3)

Ret = Percent retained on skin (%)

$$CADD = \frac{AR \times \frac{SA}{BW} \times FQ_{cr} \times FR_{abs} \times Dil \times ED_{cr} \times CF_1}{AT_{cr} \times CF_2}$$

Where:

$CADD$ = Potential Chronic Average Daily Dose ($\text{mg}/\text{kg}\text{-day}$)

AR = Amount retained on the skin ($\text{g}/\text{cm}^2\text{-event}$)

$\frac{SA}{BW}$ = Surface area to body weight ratio (cm^2/kg)

FQ_{cr} = Frequency of use, chronic (events/year)

FR_{abs} = Absorption fraction (unitless)

Dil = Product dilution fraction (unitless)

ED_{cr} = Exposure duration, chronic (years)

CF_1 = Conversion factor (1000 mg/g)

AT_{cr} = Averaging time, chronic (years)

CF_2 = Conversion factor (365 days/year)

$$ADR = \frac{AR \times \frac{SA}{BW} \times FQ_{ac} \times FR_{abs} \times Dil \times ED_{ac} \times CF_1}{AT_{ac}}$$

Where:

ADR = Potential Acute Dose Rate ($\text{mg}/\text{kg}\text{-day}$)

AR = Amount retained on the skin ($\text{g}/\text{cm}^2\text{-event}$)

$\frac{SA}{BW}$ = Surface area to body weight ratio (cm^2/kg)

FQ_{ac} = Frequency of use, acute (events/day)

FR_{abs} = Absorption fraction (unitless)

Dil = Product dilution fraction (unitless)

ED_{ac} = Exposure duration, acute (days)

CF_1 = Conversion factor (1000 mg/g)

AT_{ac} = Averaging time, acute (days)

DER02: Product Applied to Skin (Permeability Method)

Absorbed dermal exposure can also be calculated using the permeability coefficient method and assuming a constant supply of the product on the skin throughout the exposure duration. The current version of CEM provides an estimator for a chemical-specific permeability coefficient. A permeability coefficient can be chosen by one of two methods:

1. Entering a permeability coefficient
2. Using the “Estimate” button and having the model calculate the permeability coefficient using the following equation ([U.S. EPA, 1992](#)):

$$\log(K_p) = -2.72 + 0.71(\log(K_{ow})) - 0.0061(MW)$$

$$K_p = 10^{(-2.72+0.71 \times \text{Log}K_{ow}-0.0061 \times MW)}$$

Where:

- K_p = Permeability coefficient (cm/hr)
 K_{ow} = Octanol/water partition coefficient (unitless)
 MW = Molecular weight (g/mol)

$$CADD = \frac{K_p \times D \times Dil \times Den \times \frac{SA}{BW} \times FQ_{cr} \times WF \times ED_{cr} \times CF_1}{AT_{cr} \times CF_2}$$

Where:

- $CADD$ = Potential Chronic Average Daily Dose (mg/kg-day)
 K_p = Permeability coefficient (cm/hr)
 D = Duration of use (hr/event)
 Dil = Product dilution fraction (unitless)
 Den = Density of formulation (g/cm³)
 $\frac{SA}{BW}$ = Surface area to body weight ratio (cm²/kg)
 FQ_{cr} = Frequency of use, chronic (events/year)
 ED_{cr} = Exposure Duration, chronic (years)
 WF = Weight fraction of chemical in product (unitless)
 CF_1 = Conversion factor (1000 mg/g)
 AT_{cr} = Averaging time – chronic (years)
 CF_2 = Conversion factor (365 days/year)

$$ADR = \frac{K_p \times D \times Dil \times Den \times \frac{SA}{BW} \times FQ_{ac} \times WF \times ED_{ac} \times CF_1}{AT_{ac}}$$

Where:

- ADR = Potential Acute Dose Rate (mg/kg-day)
 K_p = Permeability coefficient (cm/hr)

- D* = Duration of an event (hr/event)
- Dil* = Product dilution fraction (unitless)
- Den* = Density of formulation (g/cm³)
- $\frac{SA}{BW}$ = Surface area to body weight ratio (cm²/kg)
- FQ_{ac}* = Frequency of use, acute (events/day)
- ED_{ac}* = Exposure Duration, acute (days)
- WF* = Weight fraction of chemical in product (unitless)
- CF₁* = Conversion factor (1000 mg/g)
- AT_{ac}* = Averaging time, acute (days)

DER03: Article where Skin Contact Occurs

For articles that come into direct contact with the skin, the potential dermal dose is estimated by the following equations ([ECETOC, 2012](#); [U.S. EPA, 2012b](#); [Delmaar et al., 2005](#)). The model estimates a chemical concentration on the surface of the article that is the weight fraction of the chemical, multiplied by the density and thickness of the contact layer. The model then assumes a fraction of the chemical of the surface is available for transfer (the dislodgable fraction) and multiplies this by a transfer coefficient as well as adjustments for the fraction of contact that occurs with the article of interest.

$$CADD = \frac{WF \times Den \times CT \times TC \times FR_{aw} \times FR_{con} \times FR_{dis} \times ED_{cr} \times CF_1 \times CF_2}{BW \times AT_{cr}}$$

Where:

- CADD* = Potential Chronic Average Daily Dose (mg/kg-day)
- WF* = Weight fraction of chemical in product (unitless)
- Den* = Density of formulation (g/cm³)
- CT* = Thickness of contact layer (cm)
- TC* = Transfer coefficient (cm²/hr)
- FR_{aw}* = Fraction of time awake in environment (unitless)
- FR_{con}* = Fraction of contact that is with article of interest (unitless)
- FR_{dis}* = Fraction of chemical on surface that is dislodgable (unitless)
- ED_{cr}* = Exposure duration, chronic (years)
- CF₁* = Conversion factor (1000 mg/g)
- CF₂* = Conversion factor (24 hrs/day)
- BW* = Body weight (kg)
- AT_{cr}* = Averaging time, chronic (years)

$$ADR = \frac{WF \times Den \times CT \times TC \times F_{raw} \times ED_{ac} \times CF_1 \times CF_2}{BW \times AT_{ac}}$$

Where:

- ADR* = Potential Acute Dose Rate (mg/kg-day)
WF = Weight fraction of chemical in product (unitless)
Den = Density of formulation (g/cm³)
CT = Thickness of contact layer (cm)
TC = Transfer coefficient (cm²/hr)
F_{raw} = Fraction of time awake in environment (unitless)
ED_{ac} = Exposure duration, acute (days)
CF₁ = Conversion factor (1000 mg/g)
CF₂ = Conversion factor (24 hrs/day)
BW = Body weight (kg)
AT_{ac} = Averaging time, acute (days)

DER04: Article with Direct Transfer from Vapor Phase to Skin

Chemicals within the vapor phase can partition directly to the skin, resulting in dermal exposure. In this screening model, this process is captured by first calculating the steady state dermal load or skin surface lipid loading of the chemical of interest that would be reached if the skin were in equilibrium with the gas phase concentration. This is based on the gas-lipid partitioning coefficient that can be estimated from the *K_{ow}*, Henry's law constant, the Universal Gas Law constant, and temperature. This loading is then used to estimate the average daily dose, using methodology adapted from ([Weschler and Nazaroff, 2012](#)):

$$K_{p_cw} = 10^{(0.7 \times \text{Log}K_{ow} - 0.0722 \times MW^{\frac{2}{3}} - 5.252)}$$

$$K_{p_w} = \frac{K_{p_cw}}{1 + (K_{p_cw} \times MW^{0.5})/2.6}$$

$$K_{p_b} = \frac{K_{p_w}}{40.9 \times H}$$

$$K_{p_g} = \left(\frac{1}{V_d} + \frac{1}{K_{p_b}} \right)^{-1}$$

Where:

- K_{p_cw}* = Permeability coefficient through stratum corneum of an SVOC when the species concentration is measured in water in contact with skin (m/h)
K_{ow} = Octanol-water partition coefficient (unitless)
MW = Molecular weight (g/mol)
K_{p_w} = Permeability coefficient through the stratum corneum/viable epidermis composite of SVOC when the species concentration is measured in water in contact with skin (m/h)

- K_{p_b} = Permeability coefficient that describes the transport of a gas-phase SVOC from the boundary layer at the skin surface (b) through the stratum corneum/viable epidermis composite to dermal capillaries (m/h)
- H = Henry's law coefficient (atm/M)
- K_{p_g} = Indoor air transdermal permeability coefficient that describes transport of a gas-phase SVOC from air in the core of a room through the boundary layer adjacent to skin and then through the stratum corneum/viable epidermis composite to dermal capillaries (m/h)
- V_d = Deposition velocity (m/h)

$$DerFlux = \frac{K_{p_g} \times C_g}{CF}$$

Where:

- $DerFlux$ = Dermal flux ($\mu\text{g}/\text{cm}^2\text{-hr}$)
- K_{p_g} = Transdermal permeability coefficient (m/hr)
- C_g = Average gas phase concentration ($\mu\text{g}/\text{cm}^3$)
- CF = Conversion factor ($10000 \text{ cm}^2/\text{m}^2$)

$$\log(K_{l_g}) = 0.74 + \log(K_{ow}) + \log(H) + \log(RT)$$

Where:

- K_{l_g} = Gas-phase to skin lipid partitioning coefficient
- K_{ow} = Octanol-water partitioning coefficient
- H = Henry's Law Coefficient
- R = Universal Gas Law constant (0.0821 atm/M/K)
- T = Temperature (K)

$$CADD = \frac{DerFlux \times \frac{SA}{BW} \times \text{FracTime} \times ED_{cr} \times CF_1}{AT_{cr} \times CF_2}$$

Where:

- $CADD$ = Potential Chronic Average Daily Dose (mg/kg-day)
- $DerFlux$ = Dermal flux ($\text{g}/\text{cm}^2\text{-hr}$)
- $\frac{SA}{BW}$ = Surface area to body weight ratio (cm^2/kg)
- FracTime = Fraction of time in environment (unitless)
- ED_{cr} = Exposure duration, chronic (years)
- CF_1 = Conversion factor (24 hrs/day)

AT_{cr} = Averaging time, chronic (years)

CF_2 = Conversion factor (1000 ug/mg)

$$ADR = \frac{DerFlux \times \frac{SA}{BW} \times FracTime \times ED_{ac} \times CF_1}{AT_{ac} \times CF_2}$$

Where:

ADR = Potential Acute Dose Rate (mg/kg-day)

$DerFlux$ = Dermal flux (g/cm²-hr)

$\frac{SA}{BW}$ = Surface area to body weight ratio (cm²/kg)

$FracTime$ = Fraction of time in environment (unitless)

ED_{ac} = Exposure Duration, acute (days)

CF_1 = Conversion factor (24 hrs/day)

AT_{ac} = Averaging time, acute (days)

CF_2 = Conversion factor (1000 ug/mg)

4. Areas for Future Enhancements

Despite the enhanced versatility of CEM, there are several exposure pathways that are not yet considered.

Exposure Metrics for Short-term, Chronic, and Lifetime Exposure

Throughout the user guide and beta version of CEM, EPA provide metrics of Acute Dose Rates that are averaged over one day, and Chronic Average Daily Doses that are averaged over one year. EPA is planning to incorporate lifetime average daily doses. Further consideration could be given to additional short-term and longer-term exposure metrics. One or more metrics may be more appropriate depending on the exposure scenario and chemical of interest.

For short-term metrics, one approach could be to define a standard time period or to allow the length of an exposure event to vary. Some products may result in relatively higher and shorter lived concentrations during use. In such instances, an averaging time of <24 hours may be appropriate. A per event average or an 8 hour time weighted average could be considered. Other products may result in relatively lower and longer lived concentrations during and after use. In such instances, a per-event averaging time could be considered that is longer than one day. However, for both shorter and longer emitting products, some consideration could be given as to when to “stop” an event. Modeled air concentrations will continue to be estimated over time getting closer and closer to zero and likely below the level of quantification in air for many chemicals (for example, <1E-5 ug/m3). Applying a uniform value to “stop” an event across chemicals/scenarios such as 0.001 ug/m3 or 1 ng/m3 could be considered.

For longer-term metrics, EPA is also planning to integrate Lifetime Average Daily Doses, as included in the current version of CEM. To consider Lifetime Average Daily Dose, the duration of years of product use is considered and divided by the lifetime of use. Some products are likely used every year of an adult’s lifetime while other products may be used less frequently. For inhalation scenarios, a factor to consider is how long air concentrations remain elevated during and after product use (hours, days, weeks) alongside the frequency of use (number of events in a year) and the number of years a product is used. If enough time passes in between events (months), it may be more appropriate to consider

those exposures one at a time and use chronic average daily dose estimates. However, if exposures are more continuous (a larger percentage of the year is covered by elevated concentrations) lifetime average daily doses would be appropriate and should be considered.

Articles in Routine Contact with Water

Water facilitates migration of chemicals from articles (i.e. additives in PVC drinking water pipes, bath and pool toys, etc). However, the migration rate and environmental conditions influencing migration are not well known. Human interaction with these articles may result in exposure through hand-to-mouth and object-to-mouth contact with the surface of the article or through ingestion of water into which the chemical additive has leached. In addition, there is potential for release to the environment through down-the-drain applications. EPA is piloting a method to investigate the migration rate of chemical additives from polymers when they are in contact with water, and may consider this exposure pathway.

Products Intended to go Down the Drain

EPA currently incorporates a top-down approach based on national production volume to estimate releases from products that are intended to go down the drain by assuming that 100% of the intended production volume goes down the drain. An alternative approach is to consider the mass per use, frequency of use, fraction of the population that uses the product, per capita wastewater flow, POTW removal rate, and river dilution factors. In the future, EPA could incorporate both of these approaches for down-the-drain estimates into CEM. The mass of product per use, weight fraction of chemical in the product, and frequency per use are common inputs used in other consumer exposure models to estimate human exposure. The per capita wastewater flow and river dilution factors are highly variable across the country while the fraction of the population that uses a given product is not well characterized.

$$C = \left[\frac{M \times WF \times F \times N \times CF}{Q} \right] \times R \times SDF$$

- C = Concentration in river water (unitless)
- M = Mass per use (grams)
- WF = Fraction of chemical in the product (unitless)
- F = Frequency (uses/day/person)
- N = Fraction of population that uses the product (unitless)
- CF = Conversion factor (1000 mg/g)
- CF = Per capita wastewater flow (liters/person/day)
- R = POTW Removal Rate
- SDF = Stream Dilution Factor

Vector-Facilitated Releases from Articles Not Intended to go Down the Drain

There is emerging literature that suggests that additives that are released from Articles may be transported within indoor environments and these airborne or settled particles may become entrained on vectors like clothing and other textiles before being washed down the drain through routine laundering activities. This exposure pathway requires further investigation of the greywater of buildings as an integrated source of chemicals released down the drain. Detected chemicals that are not present in products and only present in articles present an opportunity to consider source apportionment. One potential source could be the loading (mass per surface area) of textiles and estimates of total mass of chemical per wash and number of washes per week. Another potential source could be mopping or wet-

vacuuming floors which contain settled dust of the chemical. Another potential source is the excretion of chemicals from individuals after intake occurs (for example through dust ingestion). There may be other sources that have not been considered as well. It should be noted that literature is emerging in this area and all exposure pathways are presented as potential in nature.

Products that Spill or Leak Over Time

Some liquid products intended to be applied within machinery or other appliances may get spilled during application. Additionally, some amount of the liquid may leak from the equipment over time. Examples include refrigerants or cooling agents used in appliances and motor oils that are used for vehicles and other machinery. These spills and leaks could be considered both in the context of potential human exposure as well as releases to the environment. There are existing industrial hygiene models that quantify exposures after small spills, however, how various liquid consumer products may spill or leak over time based on routine use patterns associated with equipment or appliance maintenance are not well characterized. It should be noted that the majority of these exposures are expected to be occupational. However, a small number of do-it-yourselfers and bystanders may also potentially be exposed.

Elevated Temperatures During Application and Use

Temperature is an important variable that can have a large effect on emission and migration of chemicals. For example, increased temperatures may increase the emission rate of chemicals into air leading to a faster, higher rate of emissions and using body temperature, rather than room temperature provides a better estimate of migration through mouthing. Some products and articles are heated as a routine part of use while others have variable temperatures depending on site-specific conditions of use. Temperature gradients between zones or rooms within a building can also influence interzonal air flow and air exchange rates. EPA could consider incorporating temperature within existing models or providing more guidance on how temperature influences emissions and migration in the future.

Consideration of Multiple Zones in the SVOC Article Model

While the product use models include multiple zones, the SVOC Article model does not. Given the uncertainty and variability associated with quantifying interzonal air flow and tracking of particulates across rooms, the SVOC Article model was limited to one zone at this time, under the assumption that this zone is representative of other rooms within the building. Should additional information on interzonal air flow across zones within a building and resuspension of dust across zones within a building become available, EPA could consider incorporating multiple zones.

Consideration of Chemical and/or Age-Specific Transfer Efficiencies from Surface-to-Hand, Hand-to-Mouth, and Object-to-Mouth

Transfer efficiencies are highly variable given the chemical, substrate, and human activity patterns of interest. Additional empirical data characterizing these transfer efficiencies for both children and adults would help improve model accuracy and reduce uncertainty. At present, high-end estimates based on SHEDS have been incorporated for all age groups, even though for many chemical-product and chemical-article combinations it is likely that these transfer efficiencies will be lower.

Consideration of Chemical or Material-Specific Migration Rates

Migration rates into saliva from sustained mouthing behavior are highly variable and understudied. EPA is aware of a few dozen studies that have quantified migration rates using units similar to $\mu\text{g}/\text{cm}^2/\text{hour}$. Measurements of all three parameters: mass migrated, surface area, and time are important. The reported values span several orders of magnitude and covers a range of different chemicals and substrates/materials in contact with real or artificial saliva.

EPA prefers to use experimental data for chemical of interest or a closely related analog. Additional information is needed to better characterize this important parameter. Factors that may influence the migration rate into saliva may include: size of chemical additive (molecular weight and/or molar volume); water solubility of chemical additive; chemical structure, concentration and/or loading of the chemical within the material; temperature (~37° C for human mouth), pH (~6.5 for human mouth), and composition (presences of salts, enzymes, etc.) of saliva or simulated saliva; and the type of material in contact with saliva or simulated saliva.

Consideration of Total Ingestion Rates of Indoor Dust and Particles

There is uncertainty and variability associated with quantifying the total ingestion rate of dust from all surfaces for children and adults. The total ingestion rate is variable and includes ingestion of settled dust on the floor as well as ingestion of settled dust on the surface of articles through hand-to-mouth or object-to-mouth contact, as well as ingestion of resuspended particles that are not respirable and are swallowed rather than being coughed out. In order to not overestimate, EPA is considering methodology to mechanistically capture dust ingestion across a variety of indoor sources and surfaces.

Absorbed Dermal Dose

The current version of CEM approximates absorbed dose by combining information on the permeability coefficient and a catch-all term fraction retained which accounts for removal of the chemical by all processes. Another simpler approach used by many organizations is to estimate a fraction absorbed based on physical chemical properties ([Frasch et al., 2014](#)). There are approaches which quantify absorbed dermal dose. Two of the most prominent include the IH Skin Perm and NIOSH Finite Dose Calculator. Mass absorbed is generally a function of the permeability coefficient, concentration, and exposed time plus lag time or time required to diffuse across the depth of the skin. One advantage of this approach is that it more accurately characterizes time required for absorption as well as losses that occur due to evaporation or volatilization. There are methods to estimate the mass absorbed and estimators for the necessary parameters that are based on MW, VP, Kow, and water solubility ([Frasch and Bunge, 2015](#)).

Consideration of Additional Exposure Scenarios and Exposure Defaults

EPA can always consider additional information to modify an existing exposure scenario or add new exposure scenarios as use patterns change. How exposure scenarios are defined for consumer products and articles are varied in exposure models from around the world. How consumer products are used has changed over time as formulations and methods of application evolve. Some materials are formulated directly in a home environment rather than in an industrial facility. EPA can consider newly available information on consumer exposure defaults as such information becomes available. An effort was made to review available information from multiple sources. EPA expects that additional information to better inform and refine consumer exposure scenarios will become available over time.

Glossary

Note - Values and data sources for Product and Article specific parameters are presented in Appendix B.

Acute Dose Rate; ADR (mg/kg-d) The average daily dose calculated for the 24-hour day on which the product is used. ADR is calculated with age-group specific exposure factors.

Aerosol Fraction (overspray fraction) (unitless) The portion of the product (e.g., fabric protector) that is released as an aerosol upon use. Values must be between 0 and 1. The defaults have been updated in this version of CEM to reflect newer data. Updated defaults show a 1.0 to 4.5% overspray value for aerosols (3% central tendency and 4.5% high-end) and a 3-6% overspray value for trigger sprays (4.5% central tendency and 6% high-end) ([Jayjock, 2012](#))

Air Concentration, Zone 1 (mg/m³) Estimated or user-supplied concentration of the chemical in the room in which the product or article is used.

Air Concentration, Zone 2 (mg/m³) Estimated or user-supplied concentration of the chemical in the portion of the building that is not the room in which the product or article is used.

Air Exchange Rate in Zone 1 (air exchanges/hr) The rate of the volume of air being replaced in a room divided by the volume of the room for the room or other environment where the product or article is being used [([U.S. EPA, 2011](#)) Table 19-24].

Air Exchange Rate in Zone 2 (air exchanges/hr) The rate of the volume of air being replaced in a room divided by the volume of the room for the portion of the building where there product or article is not in use [([U.S. EPA, 2011](#)) Table 19-24].

Air Exchange Rate in the Near Field (air exchanges/hr) The rate of the volume of air being replaced in the near field surrounding the product user divided by the volume of the room for the portion of the building where there product or article is not in use.

Ambient Particulate Concentration (mg/m³) Level of particulates in the outdoor environment of use or surrounding the indoor environment of use. EPA monitoring data summary information was chosen because it makes use of 570 monitors in numerous locations around the United States and represents the national trend. The central tendency value is the mean value for 2012 as presented in the Excel data that can be downloaded from the website. The low and high values are the 10th and 90th percentiles, respectively ([U.S. EPA, 2014a](#)).

Amount Retained on Skin; AR (g/cm²-event) The amount of product remaining on skin after use in the units of grams of product per square centimeter of skin area. This value is a function of film thickness (m) * density (g/cm³)* percent retained on skin. Depending on conditions of use chemicals may not be retained on skin and, for example, may be washed off. The percent retained on skin variable has been harmonized with the Amount Retained on Skin utilized by EPA's SHEDS-HT model ([Isaacs et al., 2014](#)).

Amount of Product Swallowed (g) The mass of product swallowed.

Area of Article Contact; CA (cm²) The area of an article that comes into contact with mouth or skin.

Area of Yard (m²) The area of yard that a product can be applied to the ground outdoors.

Averaging Time, Acute; AT_{ac} (days) The period over which exposures are averaged. For acute exposure assessments in CEM, the default averaging is one day for all receptors.

Averaging Time, Chronic; AT_{cr} (years) The period over which exposures are averaged. For chronic exposure assessments in CEM, the default averaging time for adults is 1 years. For children, default averaging times vary by age group.

Body Weight; BW (kg) The body weight of the receptor. Default values are from EPA's Exposure Factors Handbook (EFH).

Building Volume (m^3) The total volume of all rooms in the home or other building where the product or article is used. Building volume is use to estimate air concentrations of the chemical in Zone 2 (i.e., rooms where the product or article is not in use) [(U.S. EPA, 2011), Table 19-6].

CAS number A unique numerical identifier assigned to chemicals by the Chemical Abstracts Service. This field is automatically populated based on the chemical selected in the Scenario tab.

Chemical Migration Rate; RM ($g/m^2\cdot s$) The rate at which the chemical migrates out of an article. This input can be user-defined or calculated by other models. It is dependent on chemical properties and the type of article through which the chemical is migrating.

Chemical Name The name of the chemical. This field is automatically populated based on the chemical selected in the Scenario tab.

Chronic Average Daily Dose; $CADD$ ($mg/kg\cdot day$) The average daily dose calculated with age-group-specific exposure factors.

Cleaning Efficiency (unitless) Cleaning efficiency has a wide range of values in the literature. A literature search was conducted and values ranged from 0.05 [(Qian et al., 2008); carpets] to 0.95 [(Ewers et al., 1994); wood floors]. The values selected are:

Low: 0.05 from (Qian et al., 2008) (carpets)

Medium: 0.46 from (Yiin et al., 2002) (midpoint of range, carpets)

High: 0.95 from (Ewers et al., 1994) (wood floors)

NOTE: the high value corresponds to the most efficient cleaning (the least dusty home)

Midpoint in (Yiin et al., 2002); alternate value is midpoint in (Roberts et al., 1994); all are for carpet.

Cleaning Frequency (hr^{-1}) The rate at which the floor of a room is either vacuumed or swept. The Exposures Factors Handbook provides estimates of cleaning frequency based on self-reported cleaning frequencies. However, the mean value is very high (2 cleanings per week). For that reason, other sources of information were sought to complement this data source. After examining the data, frequencies of twice a week, once a week, and once a month were selected and converted to units of "cleanings per hour". NOTE: the high value corresponds to the most frequent cleaning (the least dusty home).

Professional judgment using data from NHAPS (Klepeis et al., 2001), the Westat survey (U.S. EPA, 1987), and "Healthy Homes" asthma intervention study (Largo et al., 2011). Also (Little et al., 2012).

Degradation Half-Life in Soil (yr) The time period for one-half of the original product mass applied to the ground to decay due to environmental fate processes.

Density of Airborne Particles; ρ_{part} (mg/m^3) Airborne particles density based on value recommended in (Little et al., 2012).

Density of Dust; ρ_{Dust} (mg/m^3) Dust density based on value recommended in (Little et al., 2012).

Density of Formulation; Den (g/cm^3) The density of the product formulation or article material. This is used by CEM for other calculations.

Density of TSP; ρ_{TSP} (mg/m^3) Density of airborne particles based on value recommended in ([Little et al., 2012](#)).

Density of Soil (mg/m^3) Density of soil used by CEM in calculating exposure from products applied to ground.

Deposition Rate, Dust; $k_{dep_{Dust}}$ (hr^{-1}) The rate at which large particulates settle from the air. The Exposure Factors Handbook provided a few different sources for deposition rates. The ([Thatcher and Layton, 1995](#)) study was chosen because it measured both deposition and resuspension rates for particles in the same house. For dust, the deposition rates for particles greater than 10 μm (10-25 and >25) were averaged and rounded to the nearest tenth [([U.S. EPA, 2011](#)); Table 19-33].

Deposition Rate, TSP; $k_{dep_{TSP}}$ (hr^{-1}) The rate at which fine particulates settle from the air. The Exposure Factors Handbook provided a few different sources for deposition rates. The ([Thatcher and Layton, 1995](#)) study was chosen because it measured both deposition and resuspension rates for particles in the same house. For TSP, the deposition rates for particles less than 10 μm (1-5 and 5-10) were averaged and rounded to the nearest tenth [([U.S. EPA, 2011](#)); Table 19-33].

Dermal Flux (cm^2/hr) Rate of transfer of a chemical through the skin per unit area.

Diffusion Coefficient (unitless) Proportionality constant between the molar flux due to molecular diffusion and the concentration gradient that describes the rate of diffusion of a chemical from a substrate. Used to model chemical behavior, specifically its migration from areas of higher concentration to areas of lower concentration consistent with Fick's Law of diffusion. If this is used in the applicable models, this value will always need to be entered by the user based on the chemical of interest.

Duration of Use, acute; D (min/use) The amount of time that a product or article is used each time it is used (i.e., per use event). CEM provides default values of this input for many products/articles. Different use durations can be used for the acute and chronic exposure assessments. For acute assessments, the duration of use must be less than 24 hours.

Duration of Use, chronic; D (min/use) The amount of time that a product or article is used each time it is used (i.e., per use event). CEM provides default values of this input for many products/articles. Different use durations can be used for the acute and chronic exposure assessments.

Dust Ingestion Rate (mg/day) Daily dust ingestion rate. Default values by age group are from EPA's Exposure Factors Handbook ([U.S. EPA, 2011](#)).

Emission Rate; ER (mg/min) The rate of release of the chemical to air upon use of the product. CEM calculates the emission rate for each 30-second time step. Users have the option to enter a constant emission rate.

NOTE: Emission Rate of dust and TSP into air and onto floor is in mg/hr (E_{ATSP} ; E_{ADust} ; E_{FTSP} ; E_{FDust}).

Evaporation Time; $EvapTime$ (min) The time required for 90% of a pure chemical film to evaporate. CEM estimates EvapTime based on the molecular weight and vapor pressure in an empirical formula developed by ([Chinn, 1981](#)).

Exposed-Skin-Contact-Area to Body Weight Ratio; $\frac{SA}{BW}$ (cm^2/kg) For articles only, the ratio of exposed skin area to body weight. Six categories are included (i.e., all body surface area; half of body surface area; 25% of face, arms, and hands; all surface area of both hands; palms and fingers of both hands; palm and fingers of one hand). The most representative category is matched to the article category.

Exposure Duration, Acute; ED_{ac} (days) The duration of product use. Not to be confused with duration of use per event. For acute assessments in CEM, the default exposure duration is one day.

Exposure Duration, Chronic; ED_{cr} (years) The duration of product use. Not to be confused with duration of use per event. For example, a spray cleaner might be used for 30 minutes per use, weekly.

Far-field volume (m^3) The portion of the use environment (Zone 1) that excludes the immediate area of product use. The concentration of the chemical in air is governed by exchange with the near-field volume. Calculated based on other values

Film Thickness; FT (cm) For products, the thickness of the layer of product remaining on the skin after use.

First-Order Emissions Decline, k (min^{-1}) First-order rate constant for the emissions decline. Calculated using the estimated time required for 90% of a film of pure chemical to evaporate (see Evaporation Time).

For the “Product Applied to a Surface Indoors Double Exponential Model” (INH02), empirical studies reported by [Wilkes et al., 1996](#)) support the assumption of 25% mass released and have estimated a relationship between the fast rate of decline (k_1) and vapor pressure, and between the slow rate of decline (k_2) and molecular weight, leading to the following “fast” and “slow” values for the rate of decline ([Evans, 1994](#)):

$$k_1 = 233.25 \times (VP \div 24) \div 60$$
$$k_2 = 0.0000584 \times (MW \div 24) \div 60$$

Fraction Absorbed (unitless) Fraction of product that is applied to the skin that is absorbed through the skin.

Fraction of Contact (unitless) Fraction of touches of all surfaces that are in contact with the article of interest.

Fraction Dislodgeable (unitless) Fraction of chemical on the surface of an object that can be dislodged and transferred to the skin by touching.

Fraction Ingested; F_{ing} (unitless) An estimate of the portion of used product or inhaled particles that are ingested. Values must be between 0 and 1. The default value is 1 and should be used unless data are available.

Fraction of Mass Emitted; f (unitless) An estimate of the portion of the chemical mass that is emitted. Values must be between 0 and 1. The default value is 0.1 and should be used unless data are available.

Fraction Organic Matter Dust (unitless) Fraction of organic matter in settled dust.

Fraction Organic Matter TSP (unitless) Fraction of organic matter in airborne particles.

Fraction of Time Spent (unitless) Fraction of day spent in a given microenvironment by receptor and activity pattern.

Frequency of Use, Acute; FQ_{ac} (events/day) The number of product or article use events per day. For acute exposure assessments, CEM estimates exposure for a single use of a product or article.

Frequency of Use, Chronic; FQ_{cr} (events/year) The number of product or article use events per year. For chronic exposure assessments, CEM provides high, medium, and low default values for many products and articles. These can be modified by the user.

Henry’s Law Coefficient (unitless) Measure of the partitioning of a chemical between air and water at equilibrium.

HVAC Penetration Efficiency for Dust (unitless) Fraction of large particulates removed from the air by the HVAC filtration system. Limited information could be found about typical HVAC filtrations. Information indicates what filtration is needed for a given rating, but the average efficiency is not usually reported. The reference was selected because it reported a typical efficiency for panel filters for small particles (0.3 to 6 μm) ([Crech et al., 1996](#)).

HVAC Penetration Efficiency for TSP (unitless) Fraction of small particulates removed from the air by the HVAC filtration system. Limited information could be found about typical HVAC filtrations. Information indicates what filtration is needed for a given rating, but the average efficiency is not usually reported. The reference was selected because it reported a typical efficiency for panel filters for “large” particles ([Creech et al., 1996](#)).

Ingestion Duration (seconds) The time during which the product is ingested. CEM provides default values for many products and articles. These can be modified by the user.

Inhalation Rate (mg/hr) The age-group-specific air inhalation rate. CEM uses separate inhalation rates for the periods during and after product use. Default values by age group are from EPA's Exposure Factors Handbook ([U.S. EPA, 2011](#)).

Inhalation Rate After Use (m³/hr) The air inhalation rate when the user is not using the product. Default values by age group are from EPA's Exposure Factors Handbook ([U.S. EPA, 2011](#)).

Inhalation Rate During Use (m³/hr) The air inhalation rate during use of the product. Default values by age group are from EPA's Exposure Factors Handbook ([U.S. EPA, 2011](#)).

Initial Concentration (mg/m³) The SVOC additive concentration in a consumer article.

Interzonal Flow Rate (m³/hr) The volumetric air flow between Zones 1 and 2 during and after product usage.

Loading (g/cm²) The amount of chemical on the surface of a mouthed article or hands that have handled articles. CEM provides default values for many products and articles. These can be modified by the user.

Mass of Product Used; *M* (g) The amount of chemical-containing product used per event. CEM provides high, medium, and low default estimates for many products. The mass of product used is multiplied by the weight fraction of the chemical in the product to calculate the amount of chemical used per event.

Mass of Product Ingested; *M_{ing}* (g) The amount of chemical-containing product ingested per event. The mass of product ingested is multiplied by the weight fraction of the chemical in the product to calculate the amount of chemical ingested per event. CEM provides default values for many products and articles. These can be modified by the user.

Molecular Weight; *MW* (g/mol) The mass of one mole of a chemical. This is needed to model chemical behavior, including emission rates. If this is used in the applicable models, this value will always need to be entered by the user based on the chemical of interest.

Near-field, far-field air exchange rate (m³/min) This input is the air exchange rate between near- and far-field areas in Zone 1 and governs the concentration of the chemical in the air of the far-field portion of the use environment.

Near-field volume (m³) The near-field volume is the portion of the use environment (Zone 1) that includes the product user and where the air concentration of the chemical is governed by emissions from product use ([Keil et al., 2009](#); [Keil and Nicas, 2003](#)).

Octanol-Air Partition Coefficient; *K_{oa}* (unitless) A physical chemical property that is used to estimate the partitioning of a chemical between a source material and air. If this is used in the applicable models, this value will always need to be entered by the user based on the chemical of interest or the user can calculate this value using EpiSuite.

Octanol-Water Partition Coefficient; *K_{ow}* (unitless) The ratio of concentrations of the chemical between octanol and water at equilibrium. If this is used in the applicable models, this value will always need to be entered by the user based on the chemical of interest or the user can calculate this value using EpiSuite.

Permeability Coefficient; K_p (cm/hr) A measure of the chemical's absorption through skin. Enter an empirical value or click the "Estimate" button to estimate the coefficient based on the chemical's molecular weight and octanol-water partition coefficient.

Porosity of Soil (unitless) A measure of the porosity, or air spaces, in soil.

Potential Event Dose; Dose (mg/kg-event) Potential dose of chemical per event, as calculated by $ING02_{kn}$ (when migration rate is known).

Potential Peak Concentration (mg/m³) The highest instantaneous air concentration that is calculated by the model during any 30-second time step, and should not be interpreted as a daily maximum concentration.

Product Dilution Fraction; Dil (unitless) The fraction of the product that is diluted. Values must be between 0 and 1.

Radius of dust particles; r_{Dust} (m) Radius of dust particles ([Little et al., 2012](#)).

Radius of TSP; r_{TSP} (m) Radius of suspended particles ([Little et al., 2012](#)).

Random Air Speed Velocity at the Near-Field Boundary (m/s) Air speed at the near-field, far-field interface of the product user ([Keil et al., 2009](#); [Keil and Nicas, 2003](#)).

Resuspension Rate, Dust (per day) The rate at which large particulates are resuspended from settled to the airborne phase. The Exposure Factors Handbook recommends resuspension rates from the Thatcher and Layton 1995 study. For dust, the deposition rates for particles greater than 10 μm (10-25 and >25) were averaged and rounded to two significant digits [([U.S. EPA, 2011](#)); Table 19-33].

Resuspension Rate, TSP (per day) The rate at which small particulates are resuspended from settled to the airborne phase. The Exposure Factors Handbook recommends resuspension rates from the ([Thatcher and Layton, 1995](#)) study. For TSP, the resuspension rates for particles less than 10 μm (0.3 to 0.5, 0.6 to 1, 1-5 and 5-10) were averaged and rounded to two significant digits [([U.S. EPA, 2011](#)); Table 19-33].

Saturation Concentration in Air (mg/m³) The concentration at which exchange between the gas and liquid phases of the chemical are at equilibrium. Air concentrations estimated by CEM or entered by the user may not be greater than the saturation air concentration. If the user does not enter a saturation air concentration, it may be estimated within CEM using the chemical's molecular weight and vapor pressure. CEM estimates the saturation air concentration at standard temperature and pressure.

Skin Partitioning Coefficients (unitless) Multiple coefficients are used to describe the partitioning of a chemical between air, lipids, and multiple layers of the skin. Each are employed within the dermal air-to-skin model (DER04).

Soil Ingestion Rate (mg/day) Daily soil ingestion rate. Default values by age group are from EPA's Exposure Factors Handbook ([U.S. EPA, 2011](#)).

Source Rate for Floor Dust (mg/hr) Amount tracked in and collected on doormat. This value is based on a study by [von Lindern et al. \(2016\)](#) that measured the amount of dirt deposited on a floor mat in homes near a Superfund site.

Although Superfund sites are expected to have higher contaminant concentrations, the assumption is made that the amount of dirt (not the amount of contaminant) is roughly the same across the United States as it is near this site. The geometric mean and geometric standard deviation across the different study regions was estimated to be 248 $\text{mg}/\text{m}^2/\text{day}$ and 2.5, respectively. The mat used in the study for dirt collection was 0.318 m^2 , so multiplying gives a geometric mean estimate of 79 mg/day in each home.

The von Lindern study estimates the amount of dirt on an entryway floor mat, but additional dirt will be tracked to the rest of the home. [Thatcher and Layton \(1995\)](#) provide an estimate of the rate of accumulation of dirt on a mat versus

the “trackable” areas in the home. Using the relative areas of the home to get the total amount of dirt tracked per week and taking the ratio, it was estimated that 13% of the tracked dirt is on the mat and 87% is in the rest of the house.

To make the final calculation, the von Lindern geometric mean of 79 mg/day was divided by 0.13 to estimate the total amount tracked into the house (610 mg/day or 25.3 mg/hr). The central tendency value is based on this estimate. The low and high values are then the 10th and 90th percentile values in the distribution using the GSD of 2.5 ([von Lindern et al., 2003](#); [Thatcher and Layton, 1995](#)).

Source Rate for Floor TSP (mg/hr) Amount tracked in and collected on doormat. Track-in likely includes both smaller (<10 um) and larger particles. However, the smaller particles likely stick better the shoe through electrostatic forces. At this time, all track-in is assumed to occur in the larger (dust) size.

Source Rate for Suspended Dust (mg/hr) Rate at which large airborne particulates are generated in an indoor environment. Dander is considered the primary dust source for particles greater than PM10. A literature search returned no scientific sources for how much dander a person sheds per day; however, several websites anecdotally quoted a number of 1.5 in 24 hours. To calculate the values for the model, we assumed a home included 2 adults that spend the median amount of time in the house (low), 2 adults and 2 children that spend the median amount of time in the house (medium), and 2 adults and 2 children that spend time in the house at the 90th percentile level (high).

The CHAD database was used to estimate the amount of time adults and children spend in the house ([U.S. EPA, 2014b](#)). Because dander is based on surface area, we assumed the “children” were under 5 years old; older children will begin to have the same surface area as their parents and should be treated as adults. These values are:

Median: adults: 16.25 23 hrs; children under 5: 21.5 hrs
 90th percentile: adults: 23 hrs; children under 5: 24 hrs

The relative surface areas of children and adults were used to estimate the typical child dander shed mass per day. The Exposure Factors Handbook provides estimates for children in different age groups and adults for each decade ([U.S. EPA, 2011](#)). The values were used to estimate the average childhood (<5) and adult (18-49) surface area by taking time-weighted averages of the values in the Handbook. The resulting values are:

Adults: 2.1 m²
 Children: 0.6 m²

The final dander shed rates are found by using the equations:

$$\text{Adults: } 1.5 \frac{g}{day} \times \text{fraction time spent} \times \text{number of adults} \times \frac{1 \text{ days}}{24 \text{ hour}} \times 1000 \frac{mg}{g}$$

$$\text{Children: } 1.5 \frac{g}{day} \times \frac{\text{child surface area}}{\text{adult surface area}} \times \text{fraction time spent} \times \text{number of adults} \times \frac{1 \text{ days}}{24 \text{ hour}} \times 1000 \frac{mg}{g}$$

Then, low, mid, and high values are estimated by the equations:

$$\text{Low} = 2 \times \text{adult median}$$

$$\text{Medium} = 2 \times \text{adult median} + 2 \times \text{child median}$$

$$\text{High} = 2 \times \text{Adult 90th} + 2 \times \text{child 90th}$$

Where “median” and “90th” refer the time spent value used. Multiple secondary sources ([Bijlsma, 2015](#); [Trimarchi, 2010](#)).

Source Rate for Suspended TSP (mg/hr) Generation rate for fine particulates inside the home. The PM₁₀ particles generated inside the home were assumed to come from two dominant sources: cooking and smoking. Other sources (e.g., candles) were not considered at this time.

For cooking, the CARB study was used because it looked at emission rates (rather than just particulate concentrations) across a wide range of cooking activities for PM10 [(CARB, 2001), Table 3-32]. The cooking rates for the different activities were averaged to give an emission rate of 352 mg/hr during the cooking event.

The Department of Energy 2009 RECS survey provides information about how many times a day a person uses a stove [(U.S. EIA, 2009), Table HC3.1]. The distribution is wide with most respondents using once a day, a few times a week, or once a week. “Low” assumes once a week and “medium” and “high” assume once a day. The duration of use per event was assumed to be one hour. The average emission rate was normalized for duration and frequency of use to give an average emission rate of 2.1 mg/h (low) and 14.7 mg/hr (medium and high).

For the “high” case, cigarette smoke was added as an additional source. (Klepeis et al., 2003) reports an average emission rate of 0.7 to 0.9 mg/min for fine particulate. We used the midpoint, 0.8 mg/min. For frequency and duration, we assumed 12 smoking events each lasting 15 minutes. Normalizing for frequency and duration gave an emission rate of 6 mg/hr. This was added to the “medium” cooking emission rate to give 20.7 mg/hr.

Surface Area of Article (m²) The surface area of articles containing the SVOC. CEM provides default values for many products and articles. These can be modified by the user. Note, the model user can assume that multiple articles are present within a single room. For example, 50 toys instead of 1 toy; 2 sofas instead of 1 sofa. However, cautions should be exercised and the model user is encouraged to think through how many articles of a given type are likely to be present throughout a building. Using a high-end number of articles and surface area exposed may provide an upper-bound, but an average number of articles and surface area exposed is likely to provide more realistic exposure estimates.

Surface Area of the Near-Field Geometry (m²) Surface area of the hemispherical bubble surrounding the product user. Surface area for a use area with a radius of r is $1/2 \cdot \pi \cdot 2 \cdot \pi \cdot r^2$ (Keil and Nicas, 2003).

Surface Area of the Indoor Environment (m²) Surface area of the indoor environment, calculated as a function of the zone volume and the surface area to volume ratio from the Exposure Factors Handbook.

SVOC Gas-Phase Concentration in Contact with Article Surface (ug/m³) For materials with an SVOC additive present at greater than 15% on a per weight basis, (Little et al., 2012) recommends using the saturation vapor pressure concentration. When the additive concentration is less than 15%, (Little et al., 2012) recommends using monitoring data to back calculate this value. Because the saturation vapor pressure concentration is the highest concentration that could be present, using this value will potentially lead to over predictions of migration. For screening purposes, CEM uses the saturation vapor pressure in the absence of any monitoring data.

SVOC Gas Phase Mass Transfer Coefficient; h (m/hr) The mass transfer coefficient for SVOCs between bulk air and surface. If this is used in the applicable models, this value will either need to be entered by the user based on the chemical of interest or estimated by CEM based on the molecular weight of the SVOC.

SVOC Dust-Air Partition Coefficient; K_{Dust} (m³/mg) The ratio of concentrations of the chemical between dust and air at equilibrium, specific to SVOCs. If this is used in the applicable models, this value will either need to be entered by the user based on the chemical of interest or estimated by CEM based on the volume fraction of organic matter in settled dust, the octanol-air partition coefficient for the particular SVOC, and the density of airborne particles. This value can also be estimated in the PARAMS model using vapor pressure.

SVOC Partition Coefficient, TSP (m³/mg) The ratio of concentrations of the chemical between total suspended particulate matter and air at equilibrium, specific to SVOCs. If this is used in the applicable models, this value will either need to be entered by the user based on the chemical of interest or estimated by CEM based on the volume fraction of

organic matter in airborne particles, the octanol-air partition coefficient for the particular SVOC, and the density of airborne particles. This value can also be estimated in the PARAMS model using vapor pressure.

Thickness of Contact Layer; CT (cm) For articles, describes the thickness of the article layer that contains the chemical of interest and is not to be confused with "Film Thickness on Skin." The default value for this input was set to 1 cm. EPA is considering article-specific default values for thickness.

Time; t (min) The time of the current time step.

Temperature (F) The temperature of the indoor environment.

Transfer Coefficient (cm^2/hr) A measure of the rate of transfer of a chemical on a surface to the skin.

Transfer Factor (unitless) An estimate of the fraction of chemical on the surface of the article transferred to skin. Values must be between 0 and 1. The default value is the highest end article to skin transfer efficiency from SHEDS should be used unless data are available.

User-defined Emission Rate (mg/min) See Emission Rate. Enter a value to prevent CEM from calculating emission rates for use in exposure estimation (inhalation exposures only).

Use Environment Floor Area (m^2) The two-dimensional floor area of Zone 1, the room or other environment where the product or article is being used.

Use Environment Volume; V (m^3) The volume of the room or other location where the product or article is being used. It is used to estimate the air concentration of the chemical in Zone 1 (i.e., the use environment) ([U.S. EPA, 2011](#)).

Vapor Pressure; VP (torr) A chemical property that represents the saturation pressure of the chemical above a solid or liquid substance. If this is used in the applicable models, this value will always need to be entered by the user based on the chemical of interest.

Volume Ingested (cm^3/event) Volume ingested is the volume of product or article ingested.

Volume of Product (mL) Volume of product used, can be diluted or undiluted.

Water Solubility (g/100 g water) The saturation mass concentration of the chemical in water at a given temperature. It also may be used as a proxy for chemical solubility in sweat or saliva. If this is used in the applicable models, this value will always need to be entered by the user based on the chemical of interest.

Weight Fraction; WF (unitless) The fraction of chemical present within a product or article. The sum of all chemicals present would equal 1. For example if a fragrance is present at 1% within a cleaning product, the weight fraction input would be 0.01. This value is user defined.

APPENDIX A: Output from INH06-ING04-ING05-DER04 and Conversion to Dose

The SVOC dust model was run for five years during beta testing to ensure the model reached steady state for all the different high, medium, and low combinations of input variables within five years. Because the model reached steady state, the following simplifying assumptions were made:

“Omnipresent article”: An article or articles of similar size (i.e., emission rate) is present in the house throughout the life of the individual. Each of these consecutive articles contain the same SVOC and in similar amounts.

Constant Lifetime Concentrations: The steady-state air phase, air particulate, and dust concentrations simulated in the model during the 5 year simulation are the approximate concentrations for *each* consecutive article (i.e., the article in place from birth to age 5, the article in place from age 5 to age 10, etc). Thus, these steady-state concentrations are the constant concentrations throughout the lifetime of the individual across all the different consecutive articles.

No Ramp Up/Ramp Down: After one article is removed and the next consecutive article is replaced, the SVOC concentration in dust from the old article decreases at approximately the same rate that the SVOC concentration in dust from the new article increases. Thus, these “ramp up” and “ramp down” phases can be neglected and the concentration can be treated as constant over the lifetime of the individual.

Steady State Conditions throughout Home: The nearly constant source of SVOCs from articles will continue over a time period that will allow for the air and dust within the house to reach steady state. Exposure will be calculated considering the whole house to be one well-mixed zone.

Based on these assumptions, the outputs of the SVOC dust model will be:

1. The steady-state air phase SVOC concentration in mg/m³,
2. The steady-state air particulate SVOC concentration in mg/g,
3. The steady-state air particulate concentration in g/m³, and
4. The steady-state effective total dust SVOC concentration in mg/g.

The 4th item is estimated as

$$TotDustConcen = \frac{FloorDustConcen \times FloorDustMass + FloorTSPConcen \times FloorTSPMass}{FloorDustMass + FloorTSPMass} \quad (A1)$$

Where:

TotDustConcen = Estimated total dust SVOC concentration, as output by the SVOC Dust model (mg/g)

FloorDustConcen = Concentration of SVOC in the floor dust (mg/g)

FloorDustMass = Mass of dust on the floor (g)

FloorTSPConcen = Concentration of SVOC in the floor TSP (mg/g)

FloorTSPMass = Mass of TSP on the floor (g)

These four different values will be used to estimate the inhalation and ingestion doses for the different age groups in the model. These are estimated as:

$$IngDose = TotDustConcen \times FracTime \times DustIngest \quad (A2)$$

Where:

IngDose = Ingestion dose of SVOC, averaged for the age group (mg/day)

TotDustConcen = Estimated total dust SVOC concentration, as output by the SVOC Dust model (mg/g)
FracTime = Age-dependent fraction of time the individual spends at home
DustIngest = Age-dependent daily ingestion rate of dust (g/day)

$$InhAirPhaseDose = AirPhaseConcen \times FracTime \times InhalRate \quad (A3)$$

Where:

InhAirPhaseDose = Inhalation dose of SVOC in the gas phase, averaged for the age group (mg/day)
AirPhaseConcen = Airphase SVOC concentration, as output by the SVOC Dust model (mg/m³)
FracTime = Age-dependent fraction of time the individual spends at home
InhalRate = Age-dependent daily inhalation rate (m³/day)

$$InhAirPartDose = AirPartConcen \times SVOCPartConcen \times FracTime \times InhalRate \quad (A4)$$

Where:

InhAirPartDose = Inhalation dose of SVOC bound to particulate, averaged for the age group (mg/day)
AirPartConcen = Particulate concentration in the air (g/m³)
SVOCPartConcen = SVOC concentration on airborne particulate (mg/g)
FracTime = Age-dependent fraction of time the individual spends at home
InhalRate = Age-dependent daily inhalation rate (m³/day)

$$InhDose = InhAirPhaseDose + InhAirPartDose \quad (A5)$$

Where:

InhDose = Total inhalation dose of SVOC, averaged for the age group (mg/day)
InhAirPhaseDose = Inhalation dose of SVOC in the gas phase, averaged for the age group (mg/day)
InhAirPartDose = Inhalation dose of SVOC bound to particulate, averaged for the age group (mg/day)

APPENDIX B: Default Inputs Tables

Default values used in CEM are provided below. Data sources for values are noted where available. Please note that professional expert judgment was also applied to *all* default value determinations.

Table B-1. Product and Article Designations, Relevant Routes of Exposure, and Relevant Models for Products and Articles

Product or Article Name	Product or Article?	Relevant Routes of Exposure			Relevant Exposure Models													
		Inhalation	Ingestion	Dermal	INH 01	INH 02	INH 03	INH 04	INH 05	INH 06	ING 01	ING 02	ING 03	ING 04	DER 01	DER 02	DER 03	DER 04
Abrasive Powder Cleaners	P	X		X	X										X	X		
Adhesive/Caulk Removers	P	X					X											
Aerosol Spray Paints	P	X		X			X								X	X		
All-purpose Liquid Cleaner (diluted)	P			X											X	X		
All-purpose Liquid Cleaner/Polish (neat)	P	X		X	X										X	X		
All-purpose Spray Cleaner	P	X		X			X								X	X		
All-purpose waxes & polishes (furniture, floor, etc)	P	X		X	X										X	X		
Anti-freeze Liquids	P																	
Anti-static Spray Fabric Protector	P	X		X			X								X	X		
Bubble Solution	P		X	X								X			X	X		
Continuous Action Air Fresheners	P	X						X										
Degreasers	P	X		X			X								X	X		
De-icing Liquids	P		X								X							
De-icing Solids	P		X								X							
Drain & Toilet Cleaners (liquid)	P			X											X	X		
Exterior Car Washes & Soaps	P	X		X			X								X	X		
Exterior Car Waxes & Polishes	P			X											X	X		
Fabric Enhancers	P			X											X	X		
Fertilizers	P		X	X							X				X	X		
Fillers & Putties	P	X		X	X										X	X		
Hand Dishwashing Soap/Liquid Detergent	P			X											X	X		
Inks Applied to Skin	P			X											X	X		
Instant Action Air Fresheners	P	X					X											

Product or Article Name	Product or Article?	Relevant Routes of Exposure			Relevant Exposure Models													
		Inhalation	Ingestion	Dermal	INH 01	INH 02	INH 03	INH 04	INH 05	INH 06	ING 01	ING 02	ING 03	ING 04	DER 01	DER 02	DER 03	DER 04
Interior Car Care Cleaning/Maintenance Products	P	X		X			X								X	X		
Lacquers & Stains	P	X		X		X									X	X		
Laundry Detergent (liquid)	P			X											X	X		
Laundry Detergent (solid/granule)	P																	
Leather Tanning, Dye, Finishing, Impregnation, & Care Products	P			X											X	X		
Liquid Body Soap	P			X											X	X		
Liquid Fuels/Motor Oil	P			X											X	X		
Liquid Hand Soap	P		X	X								X			X	X		
Liquid Photographic Processing Solutions	P	X		X		X									X	X		
Machine Dishwashing Detergent (liquid/gel)	P			X											X	X		
Machine Dishwashing Detergent (solid/granule)	P																	
One component Sealants & Caulks	P	X		X	X										X	X		
Paint Strippers/Removers	P	X		X		X									X	X		
Paints Applied to Skin (fingers, face, body)	P		X	X								X			X	X		
Shoe Polish/Wax	P			X											X	X		
Single Component Glues & Adhesives	P	X		X	X										X	X		
Soil Amendments	P		X								X							
Solid Bar Soap (body)	P			X											X	X		
Solid Bar Soap (hands)	P			X											X	X		
Solvent-based Wall Paint	P	X		X		X									X	X		
Spray Fixative (art)	P	X				X												
Spray Lubricants	P	X		X		X									X	X		
Textile Stain/Spot Removers	P	X		X	X										X	X		
Textile Finishing & Surface Treatment Products	P	X		X		X									X	X		
Textile/Fabric Dyes	P			X											X	X		

Product or Article Name	Product or Article?	Relevant Routes of Exposure			Relevant Exposure Models													
		Inhalation	Ingestion	Dermal	INH 01	INH 02	INH 03	INH 04	INH 05	INH 06	ING 01	ING 02	ING 03	ING 04	DER 01	DER 02	DER 03	DER 04
Touch-up Auto Paint	P	X		X		X									X	X		
Two-component Glues & Adhesives	P	X		X	X										X	X		
Two-component Sealants & Caulks	P	X		X	X										X	X		
Varnishes & Floor Finishes	P	X		X		X									X	X		
Vehicular/Appliance Fuels	P			X											X	X		
Water-based Wall Paint	P	X		X		X									X	X		
Whole Appliance Cleaners	P	X		X	X										X	X		
Abrasive Powder Cleaners (added to water)	P			X											X	X		
Paint Strippers/Removers (sprayed)	P	X		X		X									X	X		
Textile Finishing & Surface Treatment Products (added to water)	P			X											X	X		
Touch-up Auto Paint (sprayed)	P	X		X		X									X	X		
Fabrics, Textiles, & Apparel: Blanket/comfort object	A	X	X	X						X			X	X			X	X
Fabrics, Textiles, & Apparel: Car seat cover	A	X	X	X						X			X	X			X	X
Fabrics, Textiles, & Apparel: Clothing	A	X	X	X						X			X	X			X	X
Fabrics, Textiles, & Apparel: Curtains	A	X	X	X						X			X	X			X	X
Fabrics, Textiles, & Apparel: Fabric doll/stuffed animal	A	X	X	X						X			X	X			X	X
Fabrics, Textiles, & Apparel: Furniture cover	A	X	X	X						X			X	X			X	X
Leather Articles: Shoes/boots	A	X	X	X						X			X	X			X	X
Leather Articles: Sofa	A	X	X	X						X			X	X			X	X
Paper Articles: Disposable diapers	A	X	X	X						X			X	X			X	X
Paper Articles: Wet wipes	A	X	X	X						X			X	X			X	X
Plastic Articles: Car seat	A	X	X	X						X			X	X			X	X
Plastic Articles: Children's tents & tunnels	A	X	X	X						X			X	X			X	X
Plastic Articles: Electronics	A	X	X	X						X			X	X			X	X
Plastic Articles: Foam insulation	A	X	X	X						X			X	X			X	X

Product or Article Name	Product or Article?	Relevant Routes of Exposure			Relevant Exposure Models													
		Inhalation	Ingestion	Dermal	INH 01	INH 02	INH 03	INH 04	INH 05	INH 06	ING 01	ING 02	ING 03	ING 04	DER 01	DER 02	DER 03	DER 04
Plastic Articles: Mattress	A	X	X	X						X			X	X			X	X
Plastic Articles: Pacifier, teething, & objects intended to be mouthed	A	X	X	X						X			X	X			X	X
Plastic Articles: Sofa	A	X	X	X						X			X	X			X	X
Plastic Articles: Toy food	A	X	X	X						X			X	X			X	X
Plastic Articles: Vinyl flooring	A	X	X	X						X			X	X			X	X
Rubber Articles: Flooring	A	X	X	X						X			X	X			X	X
Rubber Articles: Toy	A	X	X	X						X			X	X			X	X
Stone, Plaster, Cement, Glass, & Ceramic: Drywall	A	X	X	X						X			X	X			X	X
Wood Articles: Bench	A	X	X	X						X			X	X			X	X
Wood Articles: Flooring	A	X	X	X						X			X	X			X	X
Wood Articles: Toy	A	X	X	X						X			X	X			X	X

^aP = Product, A = Article.

Table B-2. Default Variables Relevant to Products, Part 1

Product	Default Environment	Surface-Area-to-Body-Weight Ratio Type	Density (g/cm ³) ^a	Dilution Fraction (-)	Film Thickness (m)	Percent Retained on Skin (%)
Single Component Glues & Adhesives	Residence - Utility room	Inside of One Hand	1		0.00499	10
Two-component Glues & Adhesives	Residence - Utility room	Inside of One Hand	1			10
One component Sealants & Caulks	Residence - Living room	10% of Hand	1		0.0159	10
Two-component Sealants & Caulks	Residence - Living room	Inside of One Hand	1			10
Fillers & Putties	Residence - Bathroom	10% of Hand	1			10
Fertilizers	Outside	Both Hands	1			10
Soil Amendments	Outside	Both Hands	1			10
Instant Action Air Fresheners	Residence - Bathroom		1			

Product	Default Environment	Surface-Area-to-Body-Weight Ratio Type	Density (g/cm ³) ^a	Dilution Fraction (-)	Film Thickness (m)	Percent Retained on Skin (%)
Continuous Action Air Fresheners	Residence - Bathroom		1			
Exterior Car Waxes & Polishes	Residence - Garage	Inside of Both Hands	1.077		0.00325	10
Exterior Car Washes & Soaps	Residence - Garage	Inside of Both Hands	1	0.1		10
Interior Car Care Cleaning/Maintenance Products	Residence - Garage	Inside of One Hand	1			10
Touch-up Auto Paint	Outside	10% of Hand	1			10
All-purpose Spray Cleaner	Residence - Bathroom	10% of Hand	1			10
All-purpose Liquid Cleaner/Polish (neat)	Residence - Kitchen	Inside of One Hand	1.09		0.00214	10
All-purpose Liquid Cleaner (diluted)	Residence - Kitchen	Both Hands	1.09	0.1	0.00214	10
All-purpose waxes & polishes (furniture, floor, etc)	Residence - Living room	Inside of Both Hands	1.017		0.0021	10
Whole Appliance Cleaners	Residence - Kitchen	Inside of Both Hands	1.27			10
Drain & Toilet Cleaners (liquid)	Residence - Bathroom	Inside of Both Hands	1			10
Abrasive Powder Cleaners	Residence - Bathroom	Inside of One Hand	2			10
Anti-freeze Liquids	Residence - Garage	Inside of One Hand	1			
De-icing Liquids	Residence - Garage	Inside of One Hand	1			
De-icing Solids	Residence - Garage	Inside of One Hand	1			
Shoe Polish/Wax	Residence - Laundry room	Inside of One Hand	1			10
Textile/Fabric Dyes	Residence - Laundry room	Inside of Both Hands	1	0.1		10
Textile Finishing & Surface Treatment Products	Residence - Utility room	Both Hands	1			10
Anti-static Spray Fabric Protector	Residence - Bedroom	10% of Hand	1		0.00325	10
Leather Tanning, Dye, Finishing, Impregnation, & Care Products	Residence - Utility room	Both Hands	1			10
Vehicular/Appliance Fuels	Residence - Garage	Both Hands	0.85		0.0159	10
Inks Applied to Skin	Office	Face Hands & Arms	1			100
Laundry Detergent (liquid)	Residence - Laundry room	10% of Hand	1			10

Product	Default Environment	Surface-Area-to-Body-Weight Ratio Type	Density (g/cm ³) ^a	Dilution Fraction (-)	Film Thickness (m)	Percent Retained on Skin (%)
Laundry Detergent (solid/granule)	Residence - Laundry room	10% of Hand	1			10
Machine Dishwashing Detergent (liquid/gel)	Residence - Kitchen	10% of Hand	1.077			10
Machine Dishwashing Detergent (solid/granule)	Residence - Kitchen	10% of Hand	1			
Textile Stain/Spot Removers	Residence - Living room	Inside of One Hand	1			10
Hand Dishwashing Soap/Liquid Detergent	Residence - Kitchen	Both Hands	1	0.1	0.01	1
Fabric Enhancers	Residence - Laundry room	10% of Hand	1			10
Liquid Fuels/Motor Oil	Residence - Garage	Both Hands	0.88		0.0159	10
Spray Lubricants	Residence - Garage	10% of Hand	1		0.0159	10
Degreasers	Residence - Garage	10% of Hand	1			10
Solid Bar Soap (hands)	Residence - Bathroom	Both Hands	1		0.0159	1
Solid Bar Soap (body)	Residence - Bathroom	Whole Body	1			
Liquid Hand Soap	Residence - Bathroom	Both Hands	1			1
Liquid Body Soap	Residence - Bathroom	Whole Body	1			1
Liquid Photographic Processing Solutions	Office	Both Hands	1			10
Aerosol Spray Paints	Residence - Utility room	10% of Hand	0.9		0.00655	10
Paint Strippers/Removers	Residence - Living room	Inside of Both Hands	1		0.00188	10
Adhesive/Caulk Removers	Residence - Utility room	Inside of Both Hands	1			10
Varnishes & Floor Finishes	Residence - Utility room	Inside of Both Hands	0.88			10
Lacquers & Stains	Residence - Utility room	Inside of Both Hands	1			10
Paints Applied to Skin (fingers, face, body)	Residence - Utility room	Half Body	1			100
Spray Fixative (art)	Residence - Utility room	10% of Hand	1			
Bubble Solution	Residence - Bathroom	Inside of Both Hands	1			10
Water-based Wall Paint	Residence - Living room	Face Hands & Arms	1		0.00981	10
Solvent-based Wall Paint	Residence - Living room	Face Hands & Arms	1		0.00981	10

^a default values from various sources

Table B-3. Default Variables Relevant to Products, Part 2

Product	Level	Mass (g)	Mass Data Source	Duration (min)	Duration Data Source	Frequency (yr ⁻¹)	Frequency Data Source	Aerosol Fraction (unitless)	Aerosol Fraction Data Source
Single component glues and adhesives	High	30	(Delmaar et al., 2005) (Isaacs et al., 2014)	120	(Isaacs et al., 2014) (U.S. EPA, 1986) (ECETOC, 2012)	73	(Isaacs et al., 2014) (U.S. EPA, 1986) (ECETOC, 2012)		
	Med	10		20		52			
	Low	1		5		12			
Two-component glues and adhesives	High	250	(Delmaar et al., 2005) (Isaacs et al., 2014)	240	(ECETOC, 2012) (Isaacs et al., 2014)	14	(Isaacs et al., 2014) (Delmaar et al., 2005) (ECETOC, 2012)		
	Med	20		120		3			
	Low	2		20		1			
One component sealants and caulks	High	300	(Isaacs et al., 2014) (ECETOC, 2012) (Delmaar et al., 2005) (U.S. EPA, 1986)	120	(Isaacs et al., 2014) (ECETOC, 2012) (Delmaar et al., 2005) (U.S. EPA, 1986)	14	(Isaacs et al., 2014) (U.S. EPA, 1986) (Delmaar et al., 2005)		
	Med	150		60		3			
	Low	75		20		1			
Two component sealants and caulks	High	400	(Isaacs et al., 2014) (Delmaar et al., 2005) (ECETOC, 2012)	240	(Isaacs et al., 2014) (ECETOC, 2012) (Delmaar et al., 2005) (U.S. EPA, 1986)	14	(U.S. EPA, 1986) (Delmaar et al., 2005) (Isaacs et al., 2014)		
	Med	150		120		3			
	Low	75		20		1			
Fillers and putties	High	1000	(Isaacs et al., 2014) (Delmaar et al., 2005) (ECETOC, 2012)	240	(Isaacs et al., 2014) (Delmaar et al., 2005) (ECETOC, 2012)	14	(ECETOC, 2012) (U.S. EPA, 1986) (Delmaar et al., 2005) (Isaacs et al., 2014)		
	Med	100		60		3			
	Low	10		20		1			
Fertilizers	High	1500		150	120	4			

Product	Level	Mass (g)	Mass Data Source	Duration (min)	Duration Data Source	Frequency (yr ⁻¹)	Frequency Data Source	Aerosol Fraction (unitless)	Aerosol Fraction Data Source
	Med	1000	(U.S. EPA, 2012b)	120	(Isaacs et al., 2014)	2	(Isaacs et al., 2014)		
	Low	500	(Better Homes and Gardens, 2015)	90		1			
Soil amendments	High	350	(Isaacs et al., 2014)	90	(Isaacs et al., 2014)	14	(Isaacs et al., 2014)		
	Med	250		60		12			
	Low	150		30		3			
Instant action air fresheners	High	10	(AISE) (ECETOC, 2012) (Isaacs et al., 2014)	30	(Isaacs et al., 2014) (ECETOC, 2012) (AISE)	520	(Isaacs et al., 2014) (ECETOC, 2012) (AISE) (ACI, 2010)	0.06	(Jayjock, 2012)
	Med	8		20		365			
	Low	5		10		208		0.045	
Continuous action air fresheners	High	150	(U.S. EPA, 2007) (ECETOC, 2012)	0	(U.S. EPA, 2007) (ECETOC, 2012) (AISE)	365			
	Med	100		0		358			
	Low	50		0		351			
Exterior car waxes and polishes	High	200	(Isaacs et al., 2014)	45	(Isaacs et al., 2014)	14	(Isaacs et al., 2014) Generic Scenario		
	Med	150		30		12			
	Low	100		15		3			
Exterior car washes and soaps	High	250	(Isaacs et al., 2014)	45	(Isaacs et al., 2014)	14	(Isaacs et al., 2014)		
	Med	150		30		12			
	Low	50		15		3			
Interior car care cleaning and maintenance products	High	500	Generic Scenario	45	(U.S. EPA, 1986)	5	(U.S. EPA, 1986) (ECETOC, 2012)	0.06	(Jayjock, 2012)
	Med	325		30		3			
	Low	150		15		1		0.045	
Touch up auto paint	High	400	(Isaacs et al., 2014)	60	(Isaacs et al., 2014)	5	(Isaacs et al., 2014)	0.06	(Jayjock, 2012)
	Med	300		45		3			
	Low	200		30		1		0.045	
All-purpose spray cleaner	High	75	(Isaacs et al., 2014)	30	(Delmaar et al., 2005) (ACI)	365	(U.S. EPA, 1986)	0.06	(Jayjock, 2012)

Product	Level	Mass (g)	Mass Data Source	Duration (min)	Duration Data Source	Frequency (yr ⁻¹)	Frequency Data Source	Aerosol Fraction (unitless)	Aerosol Fraction Data Source
	Med	50		15	2010 (U.S. EPA, 1986) (Isaacs et al., 2014)	300	(U.S. EPA, 2011) (ECETOC, 2012) (AISE) (Isaacs et al., 2014)	0.045	
	Low	25		5		150			
All-purpose liquid cleaner/polish (neat)	High	300	(U.S. EPA, 2007) (ECETOC, 2012) (Delmaar et al., 2005)	30	(Delmaar et al., 2005) (U.S. EPA, 2007) (U.S. EPA, 1986) (U.S. EPA, 2011) (U.S. EPA, 1986)	365	(Isaacs et al., 2014) (U.S. EPA, 1986) (U.S. EPA, 2011) (ECETOC, 2012) (AISE)		
	Med	200		15		300			
	Low	100		5		150			
All-purpose liquid cleaner (diluted)	High	300	(U.S. EPA, 2007) (ECETOC, 2012) (Delmaar et al., 2005)	30	(Delmaar et al., 2005) (U.S. EPA, 2007) (U.S. EPA, 1986) (U.S. EPA, 2011) (U.S. EPA, 1986)	365	(Isaacs et al., 2014) (U.S. EPA, 1986) (U.S. EPA, 2011) (ECETOC, 2012) (AISE)		
	Med	200		15		300			
	Low	100		5		150			
All-purpose waxes and polishes (furniture, floor, etc)	High	80	(Isaacs et al., 2014)	60	(Delmaar et al., 2005) (U.S. EPA, 1986) (ECETOC, 2012) (U.S. EPA, 2011) (U.S. EPA, 1987) (Isaacs et al., 2014)	14	(U.S. EPA, 1986) (Delmaar et al., 2005) (ECETOC, 2012) (Isaacs et al., 2014)		
	Med	50		30		12			
	Low	30		15		3			
	High	200		30		14			

Product	Level	Mass (g)	Mass Data Source	Duration (min)	Duration Data Source	Frequency (yr ⁻¹)	Frequency Data Source	Aerosol Fraction (unitless)	Aerosol Fraction Data Source
Abrasive powder cleaners	Med	150	(Isaacs et al., 2014)	20	(Isaacs et al., 2014)	12	(Isaacs et al., 2014)		
	Low	100		10		3			
Whole appliance cleaners	High	400	(Isaacs et al., 2014)	40	(Isaacs et al., 2014)	5	(Isaacs et al., 2014)		
	Med	100		20		3			
	Low	50		10		1			
Drain and toilet cleaners (liquid)	High	300	(U.S. EPA, 2011) (Delmaar et al., 2005)	30	(Isaacs et al., 2014)	14	(Isaacs et al., 2014)		
	Med	60		20		12			
	Low	30		10		3			
	Med	50		20		52			
	Low	25		10		12			
Anti-freeze liquids	High	150		15		5			
	Med	100		10		3			
	Low	50		5		1			
De-icing liquids	High	1100	(Isaacs et al., 2014)	60	(Isaacs et al., 2014)	14	(Isaacs et al., 2014)		
	Med	1000		30		12			
	Low	900		15		3			
De-icing solids	High	1100	(Isaacs et al., 2014)	60	(Isaacs et al., 2014)	14	(Isaacs et al., 2014)		
	Med	1000		30		12			
	Low	900		15		3			
Waxes, and polishes applied to footwear (shoe polish)	High	50	(Isaacs et al., 2014)	10	(Isaacs et al., 2014)	14	(Isaacs et al., 2014)		
	Med	40		5		12			
	Low	30		3		3			
Textile (fabric) dyes	High	100	(Isaacs et al., 2014), Generic Scenario	40	(Isaacs et al., 2014)	14	(Isaacs et al., 2014)		
	Med	75		30		12			
	Low	50		20		3			
Textile/apparel finishing and impregnating/surface treatment products	High	100	(U.S. EPA, 2011)	10		5			
	Med	50		5		3			
	Low	30		3		1			
Anti-static spray fabric protector	High	75		10	(U.S. EPA, 2007) (U.S. EPA, 1986)	14	(U.S. EPA, 1986) (U.S. EPA, 2007)		

Product	Level	Mass (g)	Mass Data Source	Duration (min)	Duration Data Source	Frequency (yr ⁻¹)	Frequency Data Source	Aerosol Fraction (unitless)	Aerosol Fraction Data Source
	Med	25	Generic Scenario, (U.S. EPA, 2007)	5		7	(AISE) (ECETOC, 2012)		
	Low	10		3		2			
Leather tanning, dye, finishing, impregnation and care products	High	150	(Isaacs et al., 2014)	10	(Isaacs et al., 2014)	73	(Isaacs et al., 2014)		
	Med	135		5		52			
	Low	100		3		12			
Vehicular or appliance fuels	High	6000	(ECETOC, 2012)	30		14			
	Med	5000		20		7			
	Low	4000		10		2			
Inks applied to skin	High	15		10		14			
	Med	10		5		7			
	Low	5		3		2			
Laundry detergent (liquid)	High	400	(Isaacs et al., 2014) (U.S. EPA, 2007) (U.S. EPA, 1986) (ACI, 2010) (Delmaar et al., 2005) (ECETOC, 2012)	30	(Delmaar et al., 2005) (U.S. EPA, 2007) (U.S. EPA, 2011) (U.S. EPA, 1987) (Isaacs et al., 2014)	365	(Delmaar et al., 2005) (U.S. EPA, 2007) (ACI, 2010) (AISE) (U.S. EPA, 1986) (Isaacs et al., 2014)		
	Med	200		15		300			
	Low	75		5		185			
Laundry detergent (solid/granule)	High	200	(Isaacs et al., 2014) (U.S. EPA, 2007) (U.S. EPA, 1986) (ACI, 2010) Delmaar et al., 2005) (ECETOC, 2012)	30	(U.S. EPA, 2007) Delmaar et al., 2005) (U.S. EPA, 2011) (U.S. EPA, 1987) (Isaacs et al., 2014)	365	(Delmaar et al., 2005) (U.S. EPA, 2007) (ACI, 2010) (AISE) (U.S. EPA, 1986) (Isaacs et al., 2014)		
	Med	100		15		300			
	Low	50		5		185			

Product	Level	Mass (g)	Mass Data Source	Duration (min)	Duration Data Source	Frequency (yr ⁻¹)	Frequency Data Source	Aerosol Fraction (unitless)	Aerosol Fraction Data Source
Machine dishwashing detergent (liquid/gel)	High	40	(Isaacs et al., 2014), (ECETOC, 2012)	10	(Isaacs et al., 2014)	365	(Isaacs et al., 2014)		
	Med	20	(U.S. EPA, 2011) (ACI, 2010)	5		300			
	Low	10	(Delmaar et al., 2005)	3		185			
Machine dishwashing detergent (solid/granule)	High	20	(Isaacs et al., 2014) (ECETOC, 2012)	10	(Isaacs et al., 2014)	365	(Isaacs et al., 2014)		
	Med	10	(U.S. EPA, 2011) (ACI, 2010), Generic Scenario,	5		300			
	Low	5	(Delmaar et al., 2005)	3		185			
Stain/spot removers for fabrics and textiles	High	50	(Isaacs et al., 2014)	30	(Isaacs et al., 2014), (Delmaar et al., 2005) (AISE)	185	(Isaacs et al., 2014) (ECETOC, 2012) (U.S. EPA, 1986)		
	Med	25		20		73			
	Low	5		10		12			
Hand dishwashing soap/liquid detergent	High	125	(Isaacs et al., 2014)	30	(Isaacs et al., 2014)	365	(Isaacs et al., 2014)		
	Med	100		20		300			
	Low	75		15		185			
Fabric enhancers	High	125	Generic Scenario (ACI, 2010) (Isaacs et al., 2014)	10	(Isaacs et al., 2014)	73	(Isaacs et al., 2014)		
	Med	100		5		52			
	Low	75		3		12			
Liquid fuels/motor oil	High	6000	(ECETOC, 2012)	30	(Isaacs et al., 2014)	14	(Isaacs et al., 2014; U.S. EPA, 1986)		
	Med	5000	(Isaacs et al., 2014)	20		7			
	Low	4000	(Isaacs et al., 2014)	10		2			

Product	Level	Mass (g)	Mass Data Source	Duration (min)	Duration Data Source	Frequency (yr ⁻¹)	Frequency Data Source	Aerosol Fraction (unitless)	Aerosol Fraction Data Source
Spray lubricants	High	300	(ECETOC, 2012)	30	(Isaacs et al., 2014)	14	(Isaacs et al., 2014)	0.06	(Jayjock, 2012)
	Med	100	(U.S. EPA, 2011)	20		7		0.045	
	Low	50		10		2			
Degreasers	High	200	(U.S. EPA, 2011) (Isaacs et al., 2014)	60	(Isaacs et al., 2014)	52	(Isaacs et al., 2014) (U.S. EPA, 2011) (U.S. EPA, 1987) (ECETOC, 2012)		
	Med	100		30		14			
	Low	50		15		6			
Solid bar soap (hands)	High	5	(ACI, 2010) (Delmaar et al., 2005) (Isaacs et al., 2014)	3	(Delmaar et al., 2005) (Isaacs et al., 2014)	1095	(U.S. EPA, 2007) (ACI, 2010) (Delmaar et al., 2005), (Isaacs et al., 2014)		
	Med	3		2		760			
	Low	1		1		365			
Solid bar soap (body)	High	15	(ACI, 2010) (Delmaar et al., 2005) (Isaacs et al., 2014)	15	(Delmaar et al., 2005) (U.S. EPA, 2011) (Isaacs et al., 2014)	760	(U.S. EPA, 2007) (ACI, 2010) (Delmaar et al., 2005) (Isaacs et al., 2014)		
	Med	10		10		365			
	Low	5		5		300			
Liquid hand soap	High	10	(ACI, 2010) (Isaacs et al., 2014)	3	(Delmaar et al., 2005) (Isaacs et al., 2014)	1095	(U.S. EPA, 2007) (ACI, 2010) (Delmaar et al., 2005) (Isaacs et al., 2014)		
	Med	5		2		760			
	Low	1		1		365			
Liquid body soap	High	25	(ACI, 2010) (Delmaar et al., 2005)	15	(Delmaar et al., 2005) (U.S. EPA, 2011)	760	(U.S. EPA, 2007) (ACI, 2010) (Delmaar et al., 2005)		
	Med	15		10		365			
	Low	5		5		300			

Product	Level	Mass (g)	Mass Data Source	Duration (min)	Duration Data Source	Frequency (yr ⁻¹)	Frequency Data Source	Aerosol Fraction (unitless)	Aerosol Fraction Data Source
Liquid photographic processing solutions	High	800	Generic Scenario	480	(U.S. EPA, 1986)	14	(U.S. EPA, 1986) (ECETOC, 2012)		
	Med	700		240		7			
	Low	600		120		2			
Aerosol spray paints	High	800	(U.S. EPA, 2007) Generic Scenario, (U.S. EPA, 2011) (Delmaar et al., 2005) (Isaacs et al., 2014)	90	(Delmaar et al., 2005; U.S. EPA, 1986) (U.S. EPA, 2007) (U.S. EPA, 2011) /AbT/ (U.S. EPA, 1987) (Isaacs et al., 2014)	14	(U.S. EPA, 2007) (Delmaar et al., 2005) (U.S. EPA, 1986) (U.S. EPA, 2011) (U.S. EPA, 1987) (ECETOC, 2012) (Isaacs et al., 2014)	0.06	(Jayjock, 2012)
	Med	400		45		7			
	Low	200		15		2			
Paint strippers/removers	High	2500	(U.S. EPA, 2014c) (Delmaar et al., 2005) Generic Scenario, (Isaacs et al., 2014)	360	(U.S. EPA, 2011) (Isaacs et al., 2014)	14	(Isaacs et al., 2014) (U.S. EPA, 2011) (U.S. EPA, 1987) (Delmaar et al., 2005) (ECETOC, 2012)	0.06	(Jayjock, 2012)
	Med	1000		120		7			
	Low	250		60		2			
Adhesive/caulk removers	High	750	(Isaacs et al., 2014)	120	(Isaacs et al., 2014)	14	(Isaacs et al., 2014)	0.06	(Jayjock, 2012)
	Med	500		90		7			
	Low	100		60		2			
Varnishes and floor finishes	High	750	Generic Scenario, (Isaacs et al., 2014)	240	(Isaacs et al., 2014) (U.S. EPA, 2011) (U.S. EPA, 1986)	20	(Isaacs et al., 2014; U.S. EPA, 2011) (U.S. EPA, 1987) (U.S. EPA, 1986) (ECETOC, 2012)		
	Med	500		180		14			
	Low	250		120		7			

Product	Level	Mass (g)	Mass Data Source	Duration (min)	Duration Data Source	Frequency (yr ⁻¹)	Frequency Data Source	Aerosol Fraction (unitless)	Aerosol Fraction Data Source
Lacquers and stains	High	1000	(U.S. EPA, 2011) Generic Scenario, (Isaacs et al., 2014)	120	(U.S. EPA, 2011, 1986) (U.S. EPA, 1987) (Isaacs et al., 2014)	20	(U.S. EPA, 1986) (ECETOC, 2012) (Isaacs et al., 2014)		
	Med	500		60		14			
	Low	250		30		7			
Paints intended to be applied to the skin (finger paints, face paint, body paint)	High	25	(Delmaar et al., 2005) (U.S. EPA, 2011) (Isaacs et al., 2014)	30	(Isaacs et al., 2014)	100	(Isaacs et al., 2014)		
	Med	2.5		25		14			
	Low	1.5		20		7			
Spray fixative (art)	High	40	(Isaacs et al., 2014)	20	(Isaacs et al., 2014)	14	(Isaacs et al., 2014)	0.06	(Jayjock, 2012)
	Med	20		15		7			
	Low	10		10		2		0.045	
Bubble solution	High	30	(Isaacs et al., 2014)	45	(Isaacs et al., 2014)	52	(Isaacs et al., 2014)		
	Med	20		30		26			
	Low	10		15		14			
Water-based wall paint	High	10000	(Isaacs et al., 2014) (ACI, 2010) (U.S. EPA, 2007) Generic Scenario, (Delmaar et al., 2005) (ECETOC, 2012; U.S. EPA, 2011)	540	(Isaacs et al., 2014), (U.S. EPA, 2007) (ECETOC, 2012) (ACI, 2010) (Delmaar et al., 2005) (U.S. EPA, 1986) (U.S. EPA, 2011) (U.S. EPA, 1987)	14	(Isaacs et al., 2014) (ACI, 2010) (Delmaar et al., 2005) (U.S. EPA, 1986) (U.S. EPA, 2011) (U.S. EPA, 1987)		
	Med	4000		360		7			
	Low	2000		120		2			
Solvent-based wall paint	High	10000	(Isaacs et al., 2014) (ACI, 2010)	540	(Isaacs et al., 2014), (U.S. EPA, 2007) (ECETOC, 2012)	14	(Isaacs et al., 2014) (ACI, 2010)		

Product	Level	Mass (g)	Mass Data Source	Duration (min)	Duration Data Source	Frequency (yr ⁻¹)	Frequency Data Source	Aerosol Fraction (unitless)	Aerosol Fraction Data Source
	Med	4000	(U.S. EPA, 2007) Generic Scenario, (Delmaar et al., 2005) (ECETOC, 2012)	260	(ACI, 2010) (Delmaar et al., 2005) (U.S. EPA, 1986) (U.S. EPA, 2011)	7	(Delmaar et al., 2005) (U.S. EPA, 1986) (U.S. EPA, 2011) (U.S. EPA, 1987)		
	Low	2000	(U.S. EPA, 2011)	120		2			

Table B-4. Default Variables Relevant to Articles

Product	Default Use Environment	Surface-Area-to-Body-Weight Ratio Type	Surface Area of Article (m ²)	Density of Article (g/cm ³)
Fabrics, Textiles, & Apparel: Curtains	Residence - Bedroom	Inside of Both Hands	1.6025	1
Fabrics, Textiles, & Apparel: Fabric doll/stuffed animal	Residence - Bedroom	Inside of Both Hands	0.278	1
Fabrics, Textiles, & Apparel: Furniture cover	Residence - Bedroom	Half Body	3	1
Fabrics, Textiles, & Apparel: Blanket/comfort object	Residence - Bedroom	Face Hands & Arms	0.185	1
Fabrics, Textiles, & Apparel: Clothing	Residence - Bedroom	Whole Body	1.1789	1
Fabrics, Textiles, & Apparel: Car seat cover	Residence - Bedroom	Half Body	0.3	1
Leather Articles: Sofa	Residence - Living room	Half Body	3	1
Leather Articles: Shoes/boots	Residence - Utility room	Inside of Both Hands	0.03	1
Rubber Articles: Toy	Residence - Kitchen	Inside of Both Hands	0.005	1
Rubber Articles: Flooring	Residence - Kitchen	Half Body	27.87	1
Wood Articles: Flooring	Residence - Living room	Half Body	27.87	1
Wood Articles: Toy	Residence - Living room	Inside of Both Hands	0.005	1
Wood Articles: Bench	Residence - Living room	Half Body	0.2	1
Plastic Articles: Vinyl flooring	Residence - Kitchen	Half Body	27.87	1
Plastic Articles: Foam insulation	Residence - Living room	Inside of One Hand	100	1
Plastic Articles: Toy food	Residence - Kitchen	Inside of Both Hands	0.005	1
Plastic Articles: Children's tents & tunnels	Residence - Kitchen	Face Hands & Arms	1	1
Plastic Articles: Mattress	Residence - Living room	Whole Body	4	1
Plastic Articles: Sofa	Residence - Living room	Half Body	3	1
Plastic Articles: Pacifier, teethers, & objects intended to be mouthed	Residence - Kitchen	Inside of Both Hands	0.005	1

Product	Default Use Environment	Surface-Area-to-Body-Weight Ratio Type	Surface Area of Article (m ²)	Density of Article (g/cm ³)
Plastic Articles: Electronics	Residence - Kitchen	Inside of Both Hands	1.62	1
Plastic Articles: Car seat	Residence - Bedroom	Half Body	0.3	1
Stone, Plaster, Cement, Glass, & Ceramic: Drywall	Residence - Garage	Inside of Both Hands	61	1
Paper Articles: Disposable diapers	Residence - Living room	Face Hands & Arms	0.0929	1
Paper Articles: Wet wipes	Residence - Living room	Inside of One Hand	0.0464	1

^a (ECETOC, 2012).

^b Isaacs et al. (2014)

Table B-5. Chemical inputs Relevant to All Articles

Level	Chemical Migration Rate (mg/cm ² /hr)	Area of Article Mouthed (cm ²)	Mouthing Transfer Efficiency (-)	Thickness of Article Surface Layer (m)	Thickness of Interior Surface (m)
High	0.14	22.5	0.5	0.01	0.005
Medium	0.06	10	0.2		
Low	1e-6	1	0.1		

Table B-6. Receptor Activity Patterns

Time	Activity Pattern 1: Person stays at home for most of the day	Activity Pattern 2: Person goes to school or work for part of the day	Activity Pattern 3: Person goes to school or work for most of the day
12:00 AM	Residence - Bedroom	Residence - Bedroom	Residence - Bedroom
1:00 AM	Residence - Bedroom	Residence - Bedroom	Residence - Bedroom
2:00 AM	Residence - Bedroom	Residence - Bedroom	Residence - Bedroom
3:00 AM	Residence - Bedroom	Residence - Bedroom	Residence - Bedroom
4:00 AM	Residence - Bedroom	Residence - Bedroom	Residence - Bedroom
5:00 AM	Residence - Bedroom	Residence - Bedroom	Residence - Bedroom
6:00 AM	Residence - Bedroom	Residence - Bedroom	Residence - Bedroom
7:00 AM	Residence - Bathroom	Residence - Bathroom	Residence - Bathroom
8:00 AM	Automobile	Automobile	Automobile
9:00 AM	Work / School / COF	Work / School / COF	Work / School / COF
10:00 AM	Residence - Living Room	Work / School / COF	Work / School / COF
11:00 AM	Residence - Living Room	Work / School / COF	Work / School / COF
12:00 PM	Residence - Kitchen	Work / School / COF	Work / School / COF

1:00 PM	Outside	Outside	Work / School / COF
2:00 PM	Residence - Living Room	Residence - Living Room	Work / School / COF
3:00 PM	Residence - Living Room	Residence - Living Room	Work / School / COF
4:00 PM	Residence - Laundry/Utility/Garage	Residence - Laundry/Utility/Garage	Work / School / COF
5:00 PM	Outside	Outside	Outside
6:00 PM	Residence - Kitchen	Residence - Kitchen	Residence - Kitchen
7:00 PM	Residence - Living Room	Residence - Living Room	Residence - Living Room
8:00 PM	Residence - Living Room	Residence - Living Room	Residence - Living Room
9:00 PM	Residence - Bedroom	Residence - Bedroom	Residence - Bedroom
10:00 PM	Residence - Bedroom	Residence - Bedroom	Residence - Bedroom
11:00 PM	Residence - Bedroom	Residence - Bedroom	Residence - Bedroom

Table B-7. Surface Area to Body Weight Ratios for Receptors by Age and Area of Body Impacted

Receptor	Level	Whole Body	Half Body	Face Hands & Arms	Both Hands	Inside of Both Hands	Inside of One Hand	10% of Hand
Adult (≥21 years)	5th%ile	292.0	146.0	18.7	14.7	7.35	3.68	1.47
	Mean	245.9	122.9	15.8	12.4	6.19	3.10	1.24
	95th%ile	208.1	104.0	13.0	10.5	5.23	2.61	1.05
Youth (16-20 years)	5th%ile	305.0	152.5	17.7	13.8	6.88	3.44	1.38
	Mean	257.0	128.5	14.9	11.6	5.80	2.90	1.16
	95th%ile	215.7	107.9	12.5	9.72	4.86	2.43	0.97
Youth (11-15 years)	5th%ile	350.0	175.0	20.5	15.8	7.92	3.96	1.58
	Mean	279.9	140.0	16.4	12.7	6.34	3.17	1.27
	95th%ile	232.0	116.0	13.6	10.5	5.24	2.62	1.05
Child (6-10 years)	5th%ile	411.2	205.6	25.5	19.4	9.71	4.85	1.94
	Mean	339.6	169.8	21.1	16.0	8.02	4.01	1.60
	95th%ile	281.9	141.0	17.5	13.3	6.67	3.33	1.33
Small Child (3-5 years)	5th%ile	451.9	225.9	30.3	22.0	11.0	5.50	2.20
	Mean	408.6	204.3	27.4	19.9	9.95	4.97	1.99
	95th%ile	362.6	181.3	24.3	17.6	8.78	4.39	1.76
Infant (1-2 years)	5th%ile	489.9	244.9	37.9	24.9	12.5	6.23	2.49
	Mean	452.4	226.2	35.0	23.0	11.5	5.75	2.30
	95th%ile	421.2	210.6	32.8	21.9	10.9	5.47	2.19
Infant (<1 year)	5th%ile	560.2	280.1	90.1	29.6	14.8	7.40	2.96
	Mean	509.6	254.8	81.9	26.9	13.5	6.73	2.69
	95th%ile	472.8	236.4	42.0	24.9	12.5	6.23	2.49

Table B-8. Receptor Inputs

Receptor	Body Weight (kg)	Inhalation Rate (m ³ /day)		Mouthing Duration (min/hr)		Transfer Coefficient (cm ² /hr)		Dust Ingestion Rate (mg/day)	Soil Ingestion Rate (mg/day)	Averaging time		Exposure Duration	
		During Use	After Use	Mean	95 th Percentile	Mean	95 th Percentile			Acute (days)	Chronic (years)	Acute (days)	Chronic (years)
Adult (≥21 years)	80	0.74	0.61			6800	17000	30	20	1	1	1	1
Youth (16-20 years)	71.6	0.72	0.68			5576	13940	60	50	1	1	1	1
Youth (11-15 years)	56.8	0.78	0.63			5576	13940	60	50	1	1	1	1
Child (6-10 years)	31.8	0.66	0.5	1.1	1.1	3740	9350	60	50	1	1	1	1
Small Child (3-5 years)	18.6	0.66	0.42	8.4	8.9	2652	6630	100	50	1	1	1	1
Infant (1-2 years)	12.6	0.72	0.35	7	22	1972	4930	60	50	1	1	1	1
Infant (<1 year)	7.8	0.46	0.23	10	22.5	1564	3910	30	30	1	1	1	1

Table B-9. Environmental Inputs Relevant to all Models^a

Environment	Zone 1 Volume	Zone 1 Air Exchange Rate	Zone 2 Air Exchange Rate	Building Volume
Residence - Whole house	492	0.45	0.45	492
Residence - Bedroom	36	0.45	0.45	492
Residence - Kitchen	24	0.45	0.45	492
Residence - Bathroom	15	0.45	0.45	492
Residence - Living room	50	0.45	0.45	492
Residence - Laundry room	8	0.45	0.45	492
Residence - Utility room	20	0.45	0.45	492
Residence - Garage		0.45	0.45	492
Office	50	1.5	1.5	1400
School	50	1.5	1.5	2800
Automobile	2.4	12.5	12.5	1E+11

^a (U.S. EPA, 2011)

Table B-11. Environmental Inputs Relevant Only to ING01

Environment	Yard Area (m ²)	Soil Depth (m)	Soil Density (kg/m ³)	Soil Porosity (-)
Outdoors	1327	0.015	2600	0.2

Table B-12. Environmental Inputs Relevant Only to Model INH06-ING04-ING05-DER04

Level	TSP							Dust						Cleaning Periodicity (hr)	Cleaning Efficiency (unitless)
	Dep. Rate Constant (hr ⁻¹) ^a	Resus. Rate Constant (hr ⁻¹) ^a	Emission Rate to Indoor Air (mg/hr)	Emission Rate to Indoor Floor (mg/hr)	Filter Pen. Ratio (unitless)	Radius of Particle (m) ^b	Ambient Particle Conc.(mg/m ³) ^c	Dep. Rate Constant (hr ⁻¹) ^a	Resus. Rate Constant (hr ⁻¹) ^a	Emission Rate to Indoor Air (mg/hr)	Emission Rate to Indoor Floor (mg/hr)	Filter Pen. Ratio (unitless)	Radius of Particle (m) ^b		
Low			2.1				0.028			84.6	7.7			0.0015	0.05 ^d
Med	1	0.000026	14.7	0	0.05		0.052	3.3	0.00021	117.9	25.3	0.8		0.006	0.46 ^e
High			20.7				0.081			156.9	82.7			0.0119	0.95 ^f

^a [Thatcher and Layton \(1995\)](#)

^b [Little et al. \(2012\)](#)

^c <http://www.epa.gov/airtrends/pm.html>

^d [Qian et al. \(2008\)](#) (carpets)

^e [Yiin et al. \(2002\)](#) (midpoint of range, carpets)

^f [Ewers et al. \(1994\)](#) (wood floors)

Table B-11. Environmental Inputs Relevant Only to the Near Field – Far Field Model

Parameter	Value	Units
Near field-Far Field Air Exchange Rate	402	hr ⁻¹
Near field-Far Field Volume	0.204	m ³

Table B-12. Partitioning Coefficient Values from the Literature

EPA has compiled available measured data on material air partition coefficients from fourteen studies. Most of the available data are for VOCs, rather than SVOCs. The material-air partition coefficient can vary based on the chemical properties such as vapor pressure and mass, but also by the type of product matrix. EPA is considering additional available approaches to estimate the material-air partition coefficient for chemicals without measured data to better inform which values could be selected for screening. The values presented below will be further reviewed before citing references and incorporating as defaults into CEM. Additional measured data and/or refined estimation approaches are of interest for this model parameter.

Chemical	Product Matrix	Partitioning coefficient (K)	Source ^a
Cyclohexane	Ceiling tile	6.8	Huang (2006)2
Toluene	cellulose fibre and fibrous glass	83.2	Huang (2006)2
Rthyl acetate	cellulose fibre and fibrous glass	239.3	Huang (2006)2
Isopropyl alcohol	cellulose fibre and fibrous glass	239.3	Huang (2006)2
Methanol	cellulose fibre and fibrous glass	3.12	Huang (2006)2
Benzene	medium density board 1	190	Wang et al 2008

Chemical	Product Matrix	Partitioning coefficient (K)	Source ^a
Benzene	medium density board 2	430	Wang et al 2008
Toluene	medium density board 1	260	Wang et al 2008
Toluene	medium density board 2	470	Wang et al 2008
Xylene	medium density board 1	330	Wang et al 2008
Xylene	medium density board 2	580	Wang et al 2008
Toluene	carpet backing	6171	Bodalal 2000
Nonane	carpet backing	6216	Bodalal 2000
Nonane	vinyl floor tile	2142	Bodalal 2000
Decane	carpet backing	14617	Bodalal 2000
Decane	plywood	6948	Bodalal 2000
Decane	vinyl floor tile	13045	Bodalal 2000
Undecane	carpet backing	24255	Bodalal 2000
Undecane	vinyl floor tile	26647	Bodalal 2000
Cyclohexane	plywood	348	Bodalal 2000
Ethylbenzene	plywood	1636	Bodalal 2000
Ethylbenzene	vinyl floor tile	1920	Bodalal 2000
Water	vinyl flooring	78 ± 6.8	Cox 2001
n-Butanol	vinyl flooring	810 ± 77	Cox 2001
Toluene	vinyl flooring	980 ± 34	Cox 2001
Phenol	vinyl flooring	1.2 (± 0.30) e5	Cox 2001
n-decane	vinyl flooring	3000 ± 420	Cox 2001
n-dodecane	vinyl flooring	1.7 (± 0.03) e4	Cox 2001
n-Tetradecane	vinyl flooring	1.2 (± 0.13) e5	Cox 2001
n-Pentadecane	vinyl flooring	4.2 (± 0.38) e5	Cox 2001
Hexanal	oriented strand board	6600 ± 400	Yuan, 2007
Styrene	polysterene foam	260 ± 17	Yuan, 2007
TVOC	Particle board	3300	Yang, 2001
Hexanal	Particle board	3300	Yang, 2001
α-Pinene	Particle board	5600	Yang, 2001
Ethyl acetate	brick	186.6	Zhang, 2004
Ethyl acetate	concrete	1186.4	Zhang, 2004
Ethyl acetate	gypsum board	88.68	Zhang, 2004
Ethyl acetate	carpet	43.91	Zhang, 2004
Ethyl acetate	wall paper	3000	Zhang, 2004
n-Octane	brick	23.14	Zhang, 2004
n-Octane	concrete	61.4	Zhang, 2004
n-Octane	gypsum board	70.02	Zhang, 2004

Chemical	Product Matrix	Partitioning coefficient (K)	Source ^a
n-Octane	carpet	98.42	Zhang, 2004
n-Octane	wall paper	2000	Zhang, 2004
DEHP	vinyl flooring	2.30E+11	Xu, 2006
Chlorobenzene	Carpet	80.34	Deng et al
Ethylbenzene	Carpet	57.05	Deng et al
123-Trimethylbenzene	Carpet	28.68	Deng et al
Diethyl-hexylphthalate	Vinyl Flooring	2.75E+11	Holmgren et al 2012
Di-iso-nonyl phthalate	Vinyl Flooring	1.88E+12	Holmgren et al 2013
Diethyl-hexyl isosorbate	Vinyl Flooring	2.58E+10	Holmgren et al 2014
Diethyl-hexyladipate	Vinyl Flooring	7.37E+09	Holmgren et al 2015
1,2-Cyclohexanedicarboxylic acid di-iso-nonyl ester	Vinyl Flooring	5.66E+11	Holmgren et al 2016
TVOC	Wallpaper	3289	Kim et al 2012
TVOC	Laminate Flooring	3289	Kim et al 2013
TVOC	Particle board	3289	Wang et al 2008
Naphthalene	Polyurethane Foam	6400	Zhao et al 2004
1,2,4-Trimethylbenzene	Polyurethane Foam	440	Zhao et al 2004
Styrene	Polyurethane Foam	310	Zhao et al 2004
p-Xylene	Polyurethane Foam	130	Zhao et al 2004
Ethylbenzene	Polyurethane Foam	110	Zhao et al 2004
Chlorobenzene	Polyurethane Foam	140	Zhao et al 2004
Toluene	Polyurethane Foam	58	Zhao et al 2004
Benzene	Polyurethane Foam	19	Zhao et al 2004

^aSources to be added in next iteration.

Table B-13. Diffusion Coefficient Values from the Literature

EPA has compiled available measured data on diffusion coefficients from sixteen studies. Most of the available data are for VOCs, rather than SVOCs. The diffusion coefficient can vary based on the chemical properties such as vapor pressure and mass, but also by the type of product matrix. EPA is considering additional available approaches to estimate the diffusion coefficient for chemicals without measured data to better inform which values could be selected for screening. The values presented below will be further reviewed before citing references and incorporating as defaults into CEM. Additional measured data and/or refined estimation approaches are of interest for this model parameter.

Chemical	Product	Diffusion Coefficient (m ² /s)	Source ^a
1,2- Propanediol	Carpet	6.50E-14	Little et al. (1994)
1,2,3-Trimethylbenzene	Carpet	6.00E-11	Deng et al
1,2,4-Trimethylbenzene	Polyurethane Foam	1.00E-13	Zhao et al 2004
1,2-Cyclohexanedicarboxylic acid di-iso-nonyl ester	Vinyl Flooring	1.18E-14	Holmgren et al 2012

Chemical	Product	Diffusion Coefficient (m ² /s)	Source ^a
1,2-Dichloroethane	HPDE Geomembrane	2.60E-12	Chao et al (2006)
2,2,4-Trimethylpentane	Carpet	6.00E-15	Little et al. (1994)
2,3,5,6-Tetramethyl-phenol	Low Density Polyethylene	1.60E-13	Piringer (2008)
2,3-Benzopyrrole	Low Density Polyethylene	5.50E-13	Piringer (2008)
2,6-Di-tert-butyl-4-methyl-phenol	Low Density Polyethylene	4.80E-14	Piringer (2008)
2-Ethyl-1-hexanol	Carpet	8.80E-14	Little et al. (1994)
2-Hydroxy-4-ethandiol methyl-thioacetic acid ester ^b	Low Density Polyethylene	9.00E-15	Piringer (2008)
2-Phenyl-ethanol	Low Density Polyethylene	4.30E-13	Piringer (2008)
3,7-Dimethyl-6-octene-1-al ^b	Low Density Polyethylene	1.00E-13	Piringer (2008)
3,7-Dimethyl-octene-3-ol ^b	Low Density Polyethylene	1.60E-13	Piringer (2008)
3-Octen-2-one	Low Density Polyethylene	7.30E-13	Piringer (2008)
3-Phenyl-1-propanol	Low Density Polyethylene	2.80E-13	Piringer (2008)
4-Ethenylcyclohexene ^b	Carpet (Nylon and polypropelyne w SBR adhesive)	2.10E-12	Little et al. (1994)
4-Ethenylcyclohexene ^b	Carpet (Nylon w SBR latex adhesive)	5.20E-12	Little et al. (1994)
4-Isopropyl-toluene	Low Density Polyethylene	5.40E-13	Piringer (2008)
4-Phenylcyclohexene (PCH)	Carpet (Nylon and polypropelyne w SBR adhesive)	1.20E-12	Little et al. (1994)
4-Phenylcyclohexene (PCH)	Carpet (Nylon w SBR latex adhesive)	5.90E-13	Little et al. (1994)
4-Phenylcyclohexene (PCH)	Carpet (Nylon w SBR latex adhesive)	5.00E-13	Little et al. (1994)
7-Methyl-quinoline	Low Density Polyethylene	4.30E-13	Piringer (2008)
Acetaldehyde (ACE)	Carpet (Nylon w PVC backing)	6.40E-12	Little et al. (1994)
a-Pinene	Particle board	1.20E-10	Yang et al. (2001)
Benzene	HPDE Geomembrane	7.10E-12	Chao et al (2006)
Benzene	Low Density Polyethylene	1.10E-12	Piringer (2008)
Benzene	Low Density Polyethylene	4.00E-13	Piringer (2008)
Benzene	Polyurethane Foam	7.00E-13	Zhao et al 2004
Cedrylacetate	Low Density Polyethylene	4.10E-14	Piringer (2008)
Chlorobenzene	Carpet	1.24E-11	Deng et al
Chlorobenzene	Polyurethane Foam	3.30E-13	Zhao et al 2004
Chloroform	HPDE Geomembrane	7.90E-12	Chao et al (2006)
Cyclohexane	Ceiling Tile	2.15E-06	Farajollahi et al 2009
Cyclohexane	Plywood	1.55E-10	Bodalal et al (2000)
Decane	Carpet backing	5.42E-12	Bodalal et al (2000)
Decane	Plywood	1.28E-11	Bodalal et al (2000)

Chemical	Product	Diffusion Coefficient (m ² /s)	Source ^a
Decane	vinyl floor tile	2.09E-12	Bodalal et al (2000)
Decane	Vinyl flooring	2.10E-12	Bodalal et al (2000)
Dichloromethane	HPDE Geomembrane	1.02E-11	Chao et al (2006)
Didodecyl-3-3-thio-dipropionate	Low Density Polyethylene	2.00E-15	Piringer (2008)
Diethyl-hexyl isosorbate (isDEH) ^b	Vinyl Flooring	2.09E-14	Holmgren et al 2012
Diethyl-hexyladipate (DEHA)	Vinyl Flooring	4.48E-14	Holmgren et al 2012
Diethyl-hexylphthalate (DEHP)	Vinyl Flooring	1.75E-14	Holmgren et al 2012
Di-iso-nonyl phthalate (DINP)	Vinyl Flooring	1.33E-14	Holmgren et al 2012
Dimethyl-benzyl-carbinol	Low Density Polyethylene	7.50E-14	Piringer (2008)
Dimethyl-phthalate	Low Density Polyethylene	1.90E-13	Piringer (2008)
Diphenyl-oxide	Low Density Polyethylene	3.70E-13	Piringer (2008)
Docosane	Low Density Polyethylene	3.50E-14	Piringer (2008)
Eicosane	Low Density Polyethylene	6.30E-14	Piringer (2008)
Ethane	Low Density Polyethylene	5.40E-12	Piringer (2008)
Ethane	Low Density Polyethylene	4.80E-12	Piringer (2008)
Ethyl Acetate	Brick	2.42E-09	Zhang and Niu (2004)
Ethyl Acetate	Carpet	1.03E-08	Zhang and Niu (2004)
Ethyl Acetate	Ceiling Tile	2.01E-06	Farajollahi et al 2009
Ethyl Acetate	Concrete	4.33E-11	Zhang and Niu (2004)
Ethyl Acetate	Gypsum board	1.27E-08	Zhang and Niu (2004)
Ethyl Acetate	Wallpaper	2.78E-12	Zhang and Niu (2004)
Ethyl benzene	Carpet	1.85E-11	Deng et al
Ethyl benzene	Carpet (Nylon and polypropelyne w SBR adhesive)	1.50E-12	Little et al. (1994)
Ethyl benzene	Carpet (Nylon w SBR latex adhesive)	1.02E-11	Little et al. (1994)
Ethyl benzene	Carpet (Nylon w SBR latex adhesive)	4.30E-12	Little et al. (1994)
Ethyl benzene	HPDE Geomembrane	6.80E-12	Chao et al (2006)
Ethyl benzene	Plywood	4.04E-11	Bodalal et al (2000)
Ethyl benzene	Polyurethane Foam	3.70E-13	Zhao et al 2004
Ethyl benzene	vinyl floor tile	1.60E-11	Bodalal et al (2000)
Formaldehyde	Carpet (Nylon w PVC backing)	3.20E-12	Little et al. (1994)
Heptanol	Low Density Polyethylene	5.30E-13	Piringer (2008)
Hexanal	Oriented strand board	1.80E-12	Yuan et al. (2007)
Hexanal	Particle board	7.70E-11	Yang et al. (2001)
Limonene	Low Density Polyethylene	4.30E-13	Piringer (2008)

Chemical	Product	Diffusion Coefficient (m ² /s)	Source ^a
Methane	Low Density Polyethylene	1.90E-11	Piringer (2008)
Methane	Low Density Polyethylene	3.00E-11	Piringer (2008)
Methanol	Low Density Polyethylene	4.80E-12	Piringer (2008)
Methyl-octacosanoate	Low Density Polyethylene	3.00E-15	Piringer (2008)
Methyl-tricosanoate	Low Density Polyethylene	1.50E-14	Piringer (2008)
Naphthalene	Polyurethane Foam	6.60E-15	Zhao et al 2004
n-Butanol	Vinyl flooring	6.70E-13	Cox et al. (2001)
n-Decanal	Low Density Polyethylene	1.40E-13	Piringer (2008)
n-Decane	Vinyl flooring	4.50E-13	Cox et al. (2001)
n-Dodecane	Low Density Polyethylene	2.60E-13	Piringer (2008)
n-Dodecane	Vinyl flooring	3.40E-13	Cox et al. (2001)
n-Hexane	Ceiling Tile	1.95E-06	Farajollahi et al 2009
n-Hexane	Low Density Polyethylene	1.10E-12	Piringer (2008)
n-Hexane	Low Density Polyethylene	8.40E-13	Piringer (2008)
n-Nonanal	Low Density Polyethylene	1.80E-13	Piringer (2008)
n-Octanal	Low Density Polyethylene	2.30E-13	Piringer (2008)
n-octane	Brick	1.40E-09	Zhang and Niu (2004)
n-octane	Carpet	3.56E-08	Zhang and Niu (2004)
n-Octane	Carpet	1.69E-11	Zhang and Niu (2004)
n-octane	Concrete	1.69E-11	Zhang and Niu (2004)
n-octane	Gypsum board	1.20E-08	Zhang and Niu (2004)
n-octane	Wallpaper	4.17E-12	Zhang and Niu (2004)
Nonane	Carpet backing	2.83E-11	Bodalal et al (2000)
Nonane	Vinyl floor tile	1.48E-11	Bodalal et al (2000)
n-Pentadecane	Vinyl flooring	6.70E-14	Cox et al. (2001)
n-Pentane	Low Density Polyethylene	8.00E-13	Piringer (2008)
n-Tetradecane	Low Density Polyethylene	1.90E-13	Piringer (2008)
n-Tetradecane	Vinyl flooring	1.20E-13	Cox et al. (2001)
Octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)-propionate	Low Density Polyethylene	1.10E-15	Piringer (2008)
Octane	Ceiling Tile	1.75E-06	Farajollahi et al 2009
Phenol	Low Density Polyethylene	4.50E-13	Piringer (2008)
Phenol	Vinyl flooring	1.20E-13	Cox et al. (2001)
Propane	Low Density Polyethylene	5.20E-12	Piringer (2008)
p-Xylene	Polyurethane Foam	2.70E-13	Zhao et al 2004
Styrene	Carpet (Nylon and polypropylene w SBR adhesive)	3.10E-12	Little et al. (1994)

Chemical	Product	Diffusion Coefficient (m ² /s)	Source ^a
Styrene	Carpet (Nylon w SBR latex adhesive)	4.10E-12	Little et al. (1994)
Styrene	Carpet (Nylon w SBR latex adhesive)	3.60E-12	Little et al. (1994)
Styrene	HPDE Geomembrane	2.50E-12	Chao et al (2006)
Styrene	polysterene foam	6.20E-12	Yuan et al. (2007)
Styrene	Polyurethane Foam	1.90E-13	Zhao et al 2004
Tetradecanol	Low Density Polyethylene	8.20E-14	Piringer (2008)
Tinuvin 326	Low Density Polyethylene	2.00E-14	Piringer (2008)
Toluene	Carpet backing	4.31E-11	Bodalal et al (2000)
Toluene	HPDE Geomembrane	9.60E-12	Chao et al (2006)
Toluene	Polyurethane Foam	4.20E-13	Zhao et al 2004
Toluene	Vinyl flooring	6.90E-13	Cox et al. (2001)
Trichloroethylene	HPDE Geomembrane	1.60E-11	Chao et al (2006)
TVOC	Laminate Flooring	3.10E-13	Kim et al 2012
TVOC	Particle board	7.65E-11	Wang et al 2008
TVOC	Particle board	7.70E-11	Yang (2001)
TVOC	Wallpaper	2.00E-13	Kim et al 2012
Undecane	Carpet backing	2.79E-12	Bodalal et al (2000)
Undecane	vinyl floor tile	8.55E-13	Bodalal et al (2000)
Water	Vinyl flooring	3.60E-12	Cox et al. (2001)

^aSources to be added in next iteration.

^bChemical CAS name may be reported incorrectly in original source.

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