



# Consumer Exposure Model

**Consumer Exposure Model (CEM) Version 2.0**

## **User Guide**

**Prepared for EPA Office of Pollution Prevention and Toxics**

**by ICF**

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Disclaimer: The Consumer Exposure Model (CEM), CEM User Guide, and Appendices to the CEM User Guide have been reviewed for publication by the Risk Assessment Division of the Office of Pollution Prevention and Toxics, U.S. Environmental Protection Agency (EPA/OPPT). Approval does not signify that the contents necessarily reflect the views and policies of all Offices/Divisions in the Environmental Protection Agency, nor does the mention of trade names or commercial products constitute endorsement or recommendation for use.

## Executive Summary

US EPA's Office of Pollution Prevention and Toxics (OPPT) developed the Consumer Exposure Model (CEM). CEM is a flexible, user-friendly, and scientifically rigorous tool to rapidly assess exposure to consumer products and articles across a range of exposure scenarios and pathways. To this end, OPPT sought feedback on both the performance and ease of use of the tool through beta testing and peer review. The scenarios, chemicals, and default values currently included in CEM are based on available data and professional judgment and are presented in order for model users to conveniently and effectively use the model without determining all model inputs for each model run. Default values, chemicals, or use scenarios should be deleted, added, or refined based on newly available information. In addition, generic scenarios are available which are blank and can be populated with user-defined inputs.

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 six dermal models. All CEM models are used to estimate chemical concentrations in exposure media, including indoor air, airborne particles, settled dust, and soil. The model also evaluates 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, chronic and lifetime average daily dose of chemical resulting from product and article use scenarios associated with 73 specific product and article categories and several generic categories that can be user-defined for any product or article. 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. If measured values are not available, 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:

- 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.
- A model considering ingestion of inhaled particles that are trapped in the upper airway was added.
- An option to use products outdoors was added.
- The dermal exposure from articles model was revised to reflect CONSEXO approach and data from the OPP Residential Scenarios.

- The product applied to the ground outdoors model was revised to account for multiple product applications.
- The dermal exposure model for air-to-skin transport was revised to include a steady-state flux from the air to the skin.
- The option to specify a fraction absorbed, in addition to an absorption constant, was added to the dermal exposure models.
- 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.
- Multiple options for naming, outputting, formatting, and saving reports were added.

In response to the peer review comments, the following changes have been implemented in CEM version 2.0:

1. Product and article categories were harmonized with OECD categories. Ten new product and article categories were added to CEM. To allow for greater flexibility, six generic product categories and a generic article category were added.
2. New dermal models were added: A\_DER2 Dermal Dose from Article where Skin Contact Occurs, P\_DER2 Dermal Dose from Soil where Skin Contact with Soil or Powder Occurs. In addition, the existing dermal models were improved. The permeability coefficient,  $K_p$  of P\_DER1b was revised and a fraction absorbed estimator was incorporated into P\_DER1b. The existing A\_DER3 Dermal dose from skin contact with dust was also modified to more accurately model exposure to a chemical in dust residing on the surface of an article.
3. An abrasion term was added to the SVOC article model.
4. Functionality to account for background drinking water and soil concentrations was added.
5. The ability to report Lifetime, in addition to Chronic, Average Daily Dose, was added.
6. Maximum limits were added to restrict users from entering values beyond a reasonable value for certain inputs.
7. Model names were updated to more clearly indicate the model's function.
8. Models within CEM were compared against existing monitoring and product-testing data, where available.
9. A sensitivity analysis was completed.
10. The reports in CEM have been refined and reorganized.
11. Users can now access the User's Guide from within CEM.

## Introduction

Under the Frank R. Lautenberg Chemical Safety in the 21<sup>st</sup> Century Act amendments to (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 in combination with modeling tools where appropriate 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.

CEM contains 52 product categories and 20 article categories along with six generic product categories and one generic article category. 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 (E-FAST). 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, powdered products and products mixed with soil, direct contact with articles, 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 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 and articles. Examples include aerosol spray paints, laundry detergent, foam-based furniture, hard-plastic toys, and motor oil. Chemicals are present in products and articles 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 that provide typical weight fraction values or ranges for a given chemical present in a product or article.

Exposure scenarios combine information needed to estimate consumer exposures for a given product use. 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 coefficients, dilution factor).

There are a range of simple to complex models within CEM. The models are deterministic and appropriate for use in OPPT chemical assessments. To facilitate the ability to run scenarios quickly, each product-use category is mapped to the appropriate exposure models within CEM as shown in Table B-1. The model has been pre-parameterized with default inputs (described in Section 1) for each product use category. The product use, users, and use environment can be modified but not all inputs have complete user flexibility. For example, there are three prepopulated activity patterns for users and bystanders that can be selected.

Based on the data available, OPPT will consider variability and uncertainty associated with model estimates. Variation has been incorporated (high, moderate, and low choices) for many of the parameters that allow for estimation of central tendency and reasonable worst-case exposure estimates. Chemicals can be used in many different ways. For example, how much of a product is used (amount), how often (frequency), and for how long (duration) vary with the chemical and product. This information, when combined with human and built environment exposure factors, can be used for consumer exposure assessments. For articles, additional information on diffusion rates and other physical-chemical properties are needed to estimate emissions and subsequent exposures. Other consumer models such as CONSEXPO, MCCEM, IAQX, iSVOC, IECCU, and CONTAM provide more robust estimates of exposure, including probabilistic ranges, but also require measured data such as emission rates and emission factors derived from chamber studies. Default values are available in CEM, but the model can be run with user-defined inputs based on measured data as well. The use of measured values informed by current and robust collection of exposure data is preferred. See Section 3 for a detailed discussion of the individual consumer exposure models contained within the CEM and associated data requirements.

There are some limitations that should be considered prior to using CEM. There are a range of simple to complex models with CEM, so chemical and use specific considerations and relative data availability should be considered when selecting a model with CEM or other consumer exposure models. CEM was designed to be user friendly, with prepopulated scenarios that users can modify, however the scenarios reduce the flexibility of the model. Because CEM aims to be able to be a flexible, easy-to-access model, that can be applied to a broad suite of chemicals, as well as consumer product and article use scenarios, in both data-rich and data-poor simulations, some trade-offs were required. Notably, CEM is deterministic, rather than probabilistic, and gives point estimates of exposure for populations of interest. Within CEM, it is only possible to estimate exposure to one chemical from one product or article category in a single CEM run. Additionally, CEM is not equipped to model complex emission profiles or activity patterns of residents other than those pre-populated within CEM.

While CEM is designed to appropriately model many kinds of consumer exposure scenarios, certain fields within CEM do not have restrictions and are left to user discretion. For example, CEM does not restrict VOC models from being used with non-VOC chemicals. Because of this, some knowledge of exposure and exposure modeling is recommended when using CEM.

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
- Summary of sensitivity analyses and ground-truthing of models contained within CEM
- Areas for future enhancement
- Glossary of definitions of model parameters used in CEM

Additional CEM appendices are available on the EPA website:

- Appendix with further information on the mass-balanced article and particle model within CEM
- Appendix of model inputs used in CEM
- Appendix of sensitivity analysis results
- Appendix of ground-truthing results

# 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).<sup>1</sup> 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 2.0.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. CEM must be downloaded to a directory in which you have write permission, such as My Documents.

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). Click “Extract”. A new folder will appear where you downloaded the original zip file.

Double click the folder to open it and double click the main CEM file titled “CEM Version 2.0.accdb”.

This folder also includes a copy of this User Guide and two executable files (CEM\_NFFF\_v27.exe and SVOC14\_v3.exe).

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.

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

Inputs

- Chemical Properties
- Product/Article Properties
- Environment Inputs
- Receptor Exposure Factors
- Activity Patterns

CEM Models

Results

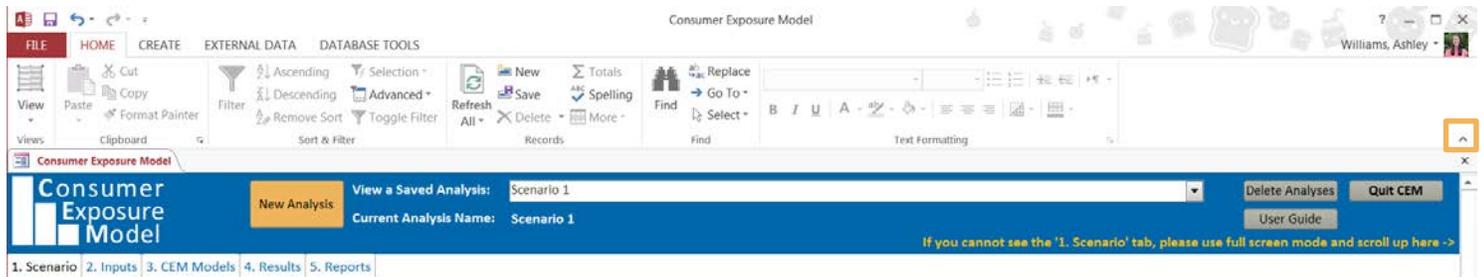
Reports

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<sup>1</sup> 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.

Instructions for using 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.

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

Additional controls on the heading bar include:

Use the ‘Delete Analyses’ button to delete one or more previously saved analyses.

‘Quit CEM’ prompts the user to save any changes to a scenario, and then closes CEM.

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	5. Reports
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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** – Enter the name of a chemical. Chemical specific information and defaults for a preselected set of chemicals can be viewed by clicking the “View Chemicals Properties” button directly above the Chemical of Interest
- 2. Product or Article Used** – First select whether to model a product or article. Then choose the product or article, and choose whether 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. There are 52 product categories and 20 article categories, which 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. There are also six generic product and one generic article category that can be used to select different models for user defined scenarios.
- 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 the receptor who uses a product directly. A bystander is a receptor who is a non-product user that 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. Only one activity pattern can be selected for a given CEM run. 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, Dust, Soil, and Drinking Water Concentrations** – In order to quickly compare exposure attributed to consumer products and articles to background exposures, user-defined background air, dust, soil, and drinking water concentrations can be specified for certain models. Background air concentrations are only associated with product inhalation models (those that utilize emission models E1-E5). Dust ingestion exposure is only associated with articles; therefore, background dust concentrations are only associated with article models (E6, A\_ING3, P\_DER2). Background drinking water concentrations are only associated with the ingestion of product swallowed, P\_ING1. Background soil concentrations are only associated with product models related to soil exposure (P\_ING2,

P\_DER2). The chronic exposure to these media are calculated and reported separately from pathway-specific exposures. These are set to zero as default.

9. **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.
10. **Exposure Pathway** – The checked boxes show which exposure model pathways will be included in the CEM run. Unchecking the box for a pathway turns off the model pathway even if it is listed in the 'Available Models' above. This allows for greater flexibility and the ability to only run a single model at a time if that is of interest.
11. **Scenario Description/Notes** – An optional free-text field to enter a scenario description for later reference. This field is output with the final report and can be used in various ways, including to track the purpose of a run, whether inputs were user supplied or estimated with CEM, data sources used for modeling runs, and other information that would be useful in later interpreting model results.
12. **Modeling Options** – Options provided for relevant models (models that do not apply will not appear). If certain pathways are not of interest, for example, ingestion exposure, they can be deselected here. 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.
13. **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 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

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	

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,
- Octanol-water partition coefficient, and
- Gas phase mass transfer 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 E6. Examples include:

Solid-phase diffusion coefficient,

Partition coefficients between air and dust, respirable particles (RP), sources, and interior surfaces (sinks), and Mass transfer coefficients to RP, 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 its development, EPA recommends the use of EpiSuite™ Version 4.11 ([U.S. EPA, 2012a](#)) to estimate physical-chemical properties if empirical data are not available. EpiSuite™ requires either the simplified molecular-input line-entry system (SMILES) code or molecular weight and vapor pressure to estimate parameters needed to CEM.

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

Saturation Concentration in Air (mg/m3): 1.10e-01 Estimate

Log Octanol-water Partition Coefficient (-): 4.59E+00

Log Octanol-air Partition Coefficient (-): 8.46E+00

**Water Solubility (mg/mL): Not Required**

Henry's Law Coefficient (atm/M): 3.31E-06

Gas Phase Mass Transfer Coefficient (m/hr): 1.75E+00 Estimate

Emission Factor (ug/m2/hr): 0.00E+00 Estimate ?

## 2.b. Product/Article Properties Input tab

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

The Product/Article Properties Input tab is used to enter required data to describe the product or article and how a receptor could interact with it. Examples include:

- Density of product/article,
- Surface area of article,
- Thickness of article surface layer,
- Product dilution factor,
- Duration of article contact, and
- Area of article mouthed.

This tab also contains data on the parameters required for dermal and ingestion exposure. More details concerning these parameters and how they are incorporated into CEM are presented in the Section 3. Examples include:

- Film thickness on skin,
- Amount retained on skin,
- Chemical migration rate,
- Thickness of contact layer,
- Surface loading,
- Mouthing transfer efficiency,
- Fraction of chemical that is dislodgable,
- Transdermal permeability coefficient,
- Absorption fraction (chronic and acute),
- Ingestion fraction (RP, dust, abraded particle),
- Chemical half-life in soil,
- Average molecule diffusion per contact,
- Frequency of article contact, and

- Adherence factor.

Additionally, this tab contains other input parameters specifically for chronic or acute assessments:

- Frequency of use,
- Duration of use, and
- Mass of product used,
- Aerosol fraction (all assessments).

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	5. Reports	
a. Chemical Properties	b. Product/Article 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.

Examples include:

- Use environment,
- Building volume,
- Use Environment volume,
- Yard area,
- Air exchange rate, Zone 1,
- Air exchange rate, Zone 2,
- Interzone ventilation rate,
- Area of interior surface, and
- Thickness of interior surface.

This tab also contains dust parameter inputs (respirable particles, dust, and abraded particle). Examples include:

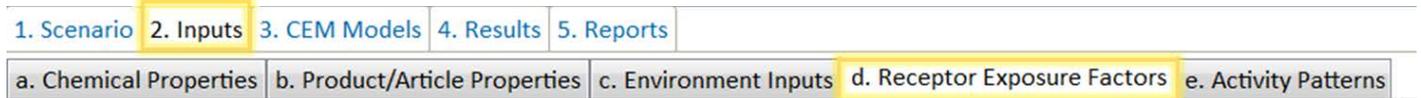
- Deposition rate (RP, dust, abraded particle),
- Resuspension rate (RP, dust, abraded particle),
- Mass generation rate, suspended (RP, dust, abraded particle),
- Mass generation rate, floor (RP, dust, abraded particle),
- Radius of particle (RP, dust, abraded particle),
- Density of particle (RP, dust, abraded particle),
- Ambient RP concentration,
- Cleaning frequency,
- Cleaning efficiency, and
- HVAC filter penetration.

Other inputs on this tab include near field inputs, and soil properties which include:

- Near-field volume
- Far-field volume
- Air exchange rate at near-field boundary, and
- Soil mixing depth,
- Soil density,
- Soil porosity,
- Concentration in soil/powders (chronic, acute).

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



The Receptor Exposure Factors Input tab is used to provide information on product or article users and incidentally exposed humans (receptors). 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.

Enter non-default values for the specific analysis under Analysis Value. For skin surface area to body weight (SA-BW) Ratio exposure factors, a drop-down menu is provided for low, medium, and high estimate values. User-specified values can also be entered. An additional table on this screen presents SA-BW Ratios for differing areas of skin exposure (e.g., whole body versus both hands), for reference.

**Choose an Exposure Factor** 1
**Receptor-specific Exposure Factors Values for this Analysis** ?

	Receptor	Default Value	Analysis Value
<b>Body Weight (kg)</b> 2	Adult (≥21 years)	3 80	4 80
Averaging Time - Chronic (years)	Youth (16-20 years)	71.6	71.6
Averaging Time - Acute (days)	Youth (11-15 years)	56.8	56.8
Exposure Duration - Chronic (years)	Child (6-10 years)	31.8	31.8
Exposure Duration - Acute (days)	Small Child (3-5 years)	18.6	18.6
Inhalation Rate After Use (m3/hr)	Infant (1-2 years)	12.6	12.6
Dust Ingestion Rate (mg/day)	Infant (<1 year)	7.8	7.8
SA-BW Ratio (cm2/kg)			
Mouthing Duration (min/hr)			
Transfer Coefficient (cm2/hr)			

## 2.e. Activity Patterns Input tab

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

CEM employs three default activity patterns, one corresponding to a person who spends 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 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	5. Reports
Model Selection	E1	P_INH1	P_DER1a	

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.

1. Scenario	2. Inputs	3. CEM Models	4. Results	5. Reports
Model Selection	E1	P_INH1	P_DER1a	
1	2			

The Model Selection sub-tab includes an option to save

intermediate estimates when running inhalation models E1-E6. Intermediate estimates include emission rates, contaminant concentrations in air, and cumulative 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. This modeling period was chosen to balance capturing total exposure from each product usage and reducing model runtime. 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.

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 E1 P\_INH1 P\_DER1a

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

E1: Emission from Product Applied to a Surface Indoors Incremental Source Model  
P\_INH1: Calculation of Inhalation Dose from Product Usage  
P\_DER1a: Dermal Dose from Product Applied to Skin, Fraction Absorbed Model

**b** Run CEM Models

**a** Option for Inhalation Models Only

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

Equations 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. 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 E1 P\_INH1 P\_DER1a

Emission from Product Applied to a Surface Indoors Incremental Source Model

$$ER(t) = M * WF * CF / ta * (1 - e^{-k(t - tstart)}) - (1 - e^{-k(t - (tstart + ta))}) * Ht$$

ER(t)	= Emission rate at time t (mg/min)	Varies
M	= Mass of product used (g)	200
WF	=Weight fraction of chemical in product (-)	1
CF	=Conversion factor (mg/g)	1000
ta	= Duration of Use (min/use)	15
k	= First-order rate constant for emissions decline (1/min)	Varies
t	= Time (min)	Varies
Ht	= 0 if t-(tstart + ta) < 0; 1 if t-(tstart + ta) > 0	Varies
tstart	= Application start time (min)	Varies

First-order rate constant, k (Eq 3-43)  
 $k [1/min] = \ln(10) / EvapTime / 60$

Evaporation time, (Eq 3-42)  
 $EvapTime [hr] = 145 / (MW * VP)^{0.9546}$

MW = Molecular Weight (g/mol)  
VP = Vapor Pressure (torr)

**Parameter Information**

Description:

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.

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 5. Reports

Cover Page Inhalation Ingestion Dermal Product/Article: All-purpose Spray Cleaner

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: (43) Aerosol Spray Paints | Chemical Name: Pentanedioic acid, dimethyl ester |  Adult (≥21 years) |  Youth (11-20 years) |  Child (<1-10 years)

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)
Lifetime	0.00E+00	2.20E-01	0.00E+00	0.00E+00	0.00E+00	2.95E-03	0.00E+00	2.23E-01
Adult (≥21 years)	2.67E+01	3.01E-01	0.00E+00	0.00E+00	2.45E-01	4.04E-03	2.69E+01	3.05E-01
Youth (16-20 years)	2.77E+01	2.74E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.77E+01	2.74E-01
Youth (11-15 years)	3.24E+01	3.20E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.24E+01	3.20E-01
Child (6-10 years)	4.59E+01	4.53E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.59E+01	4.53E-01
Small Child (3-5 years)	6.59E+01	6.51E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.59E+01	6.51E-01
Infant (1-2 years)	8.11E+01	8.01E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.11E+01	8.01E-01
Infant (<1 year)	8.61E+01	8.50E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.61E+01	8.50E-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.

## 5. Reports tab

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

Choose a Report to View

- CEM Results
- CEM Results and Inputs
- Inhalation Time-Series Graph

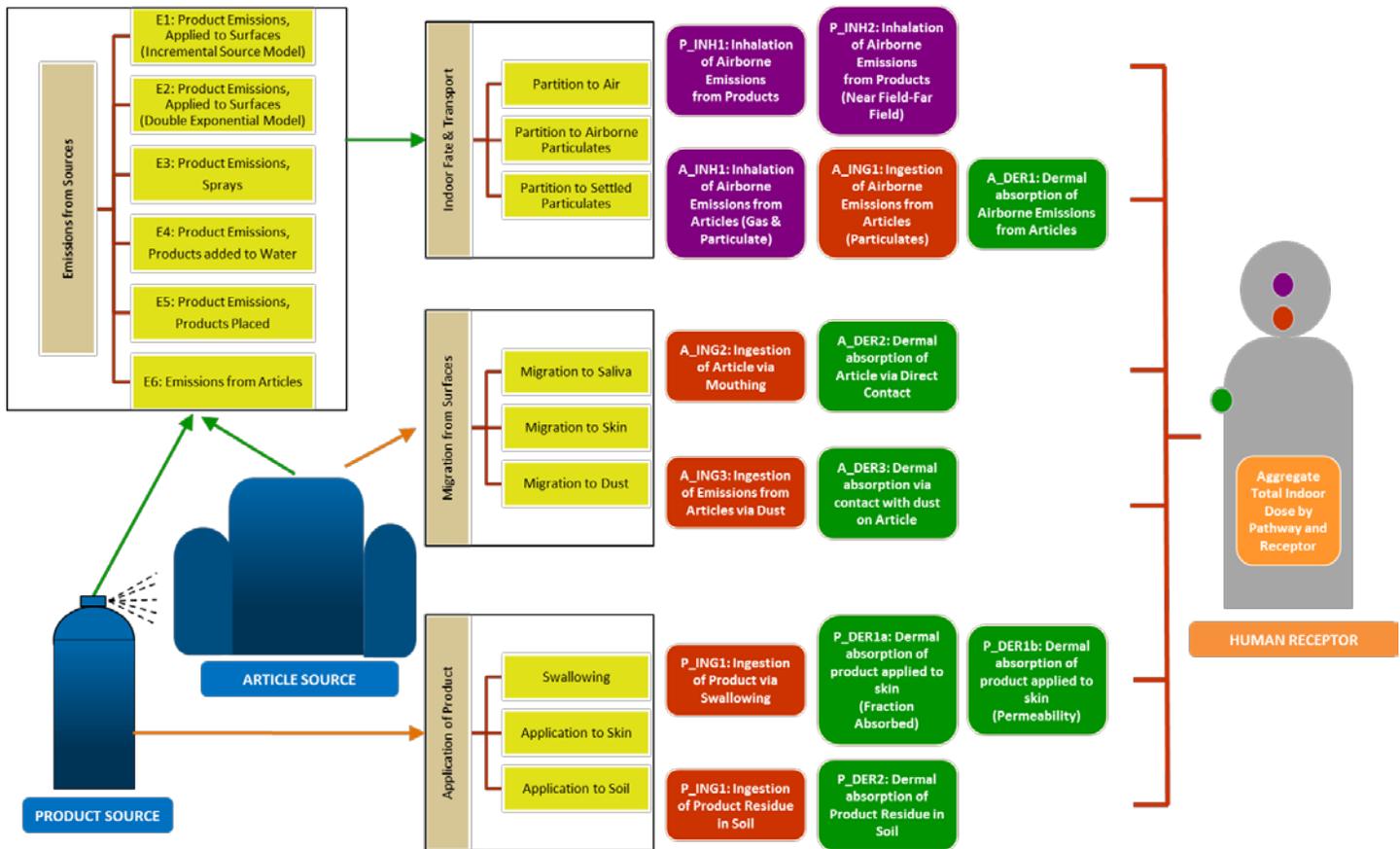
View/Save Report:

PDF/Graph

The Reports tab allows for the viewing and exportation of various reports as PDFs. Three report options are available, including the CEM Results, CEM Results and Inputs, and an Inhalation Time-Series Graph. The CEM Results report includes the results on the Cover Page and then depending on which models were run, the report includes Dermal Results, Inhalation Results, and Ingestion Results. The CEM Results and Inputs report includes all information in the CEM Results report and includes the Scenario Summary.

The Inhalation Time-Series Graph produces a Microsoft Excel file with the intermediate time-series from the inhalation model graphed and in raw data form. In order for this report to generate, the “Save intermediate estimates (increased run time)” option on the CEM Models tab must be selected.

## 2. Summary of Models within CEM



**Figure 1. Schematic relationship showing exposure models included in CEM**

**Figure 1** shows the 20 models within CEM. There are six emission models (yellow), three inhalation models (purple), five ingestion models (red), and six dermal models (green). Model names that begin with a “P” are product models and model names beginning with an “A” are article models. The following section includes brief summaries of each model included in CEM. See Section 3 for further details on model equations and parameters.

### E1: Emission from 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. This model is generally applicable to liquid products applied to surfaces that evaporate from the surfaces, such as cleaners. 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](#))

### E2: Emission from 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, and is generally appropriate for liquid products that are applied to surface and dry or cure over time, such as paints. This model assumes that 25 percent of the applied mass is released because a substantial fraction of the mass becomes trapped in the cured substrate when it dries. (Note: 10 percent of the emissions are associated with the first of the double exponential.) 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 is used 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](#))

### **E3: Emission from 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](#))

### **E4: Emission from 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). This model is appropriate for use scenarios such as laundry and dishwashing detergent. The potential duration of emissions in this case is determined from the chemical's 90 percent evaporation time. ([U.S. EPA, 2007](#))

### **E5: Emission from Product Placed in Environment**

This model is mathematically similar to E4, but is appropriate for products that are placed in the environment, but not added to water, such as air fresheners. 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](#)).

### **E6: Emission from Article Placed in Environment**

Model assumes emissions of semi-volatile organic compound (SVOC) additives from articles and subsequent partitioning between indoor air, airborne particles, settled dust, and indoor sinks 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).

### **P\_INH1: Inhalation of Product Used in Environment**

CEM predicts indoor air concentrations from product use by implementing a deterministic, mass-balance calculation utilizing an emission profile determined by implementing E1 through E5. The model uses a two-zone representation of the building of use (e.g., residence, school, office) with Zone 1 representing the room where the consumer product is used (e.g., a kitchen) and zone 2 being the remainder of the building. The product user is placed within Zone 1 for the duration of use. Otherwise, product users and bystanders follow prescribed activity patterns as described in Section 1 and inhale airborne concentrations of those zones.

## **P\_INH2: Inhalation of Product Used in Environment (Near-Field / Far-Field)**

In some instances of product use, a higher concentration of product is expected very near the product user. To model this elevated exposure, the near-field / far-field option can be selected within CEM. In this model, Zone 1 of the mass-balance model described in P\_INH01 is further divided into the near-field, with a default volume of 1m<sup>3</sup>, and far-field, the remainder of the room of use. Each zone is considered well-mixed with an air exchange between them as suggested by [Keil et al., 2009](#). The near-field can be envisioned as a bubble surrounding the user that moves throughout the room with the user, such as in the case of painting. Product users inhale airborne concentrations estimated within the near-field during the time of use and otherwise follow their prescribed activity pattern. Bystanders follow their prescribed activity pattern and inhale far-field concentrations when they are in Zone 1.

Currently, each age grouping (adult, youth, child) can only be modeled as a user or bystander within CEM. P\_INH1 and P\_INH2 can each be modeled for the same scenario and the results compared to estimate exposure by, for example, an adult user and an adult bystander.

## **A\_INH1: Inhalation from Article Placed in Environment**

CEM predicts indoor air concentrations from article exposure by implementing a deterministic, mass-balance calculation utilizing an emission profile determined by implementing E6. The model uses a one-zone representation of the building of use (e.g., residence, school, office.) As opposed to the product inhalation models, the article inhalation model tracks chemical transport between the source, air, airborne and settled particles, and indoor sinks by accounting for 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. All receptors are considered bystanders that follow prescribed activity patterns and inhale Zone 1 concentrations when they are present within the building of use.

## **P\_ING1: Ingestion of 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](#)).

## **P\_ING2: Ingestion of Product Applied to Ground Outdoors**

A shallow mixing model provides equations 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](#)).

## **A\_ING1: Ingestion after Inhalation (Article Model)**

A\_INH1 model assumes emissions of semi-volatile organic compound (SVOC) additives from articles and subsequent partitioning between indoor air, airborne particles, and settled dust over time. A\_ING1 calculates incidental ingestion of airborne particles estimated using A\_INH1 that are inhaled and trapped in the upper airway ([U.S. EPA, 2011](#))

## **A\_ING2: Ingestion of Article Mouthed**

Chemicals present in articles can be ingested by direct object-to-mouth contact, termed mouthing. The mouthing methodology relies on a migration rate of the chemical of interest from the article of interest to saliva. 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](#)).

### **A\_ING3: Incidental Dust Ingestion (Article Model)**

A\_INH1 model assumes emissions of semi-volatile organic compound (SVOC) additives from articles and subsequent partitioning between indoor air, airborne particles, and settled dust over time. A\_ING3 calculates incidental ingestion of dust contaminated with levels of SVOCs as predicted by A\_INH1 using the Tracer methodology ([U.S. EPA, 2011](#)).

### **P\_DER1a: Dermal Dose from 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 using either a permeability coefficient or fraction absorbed. This model uses a fraction absorbed to estimate dermal dose. Potential dose is the amount of a chemical contained in bulk material that is applied to the skin, represents an upper bound of exposure, and can be estimated using this model and the fraction absorbed estimator ([U.S. EPA, 2007](#); [Frasch and Bunge, 2015](#)).

### **P\_DER1b: Dermal Dose from 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. In this model, the user can specify a skin permeability coefficient if known or use the provided permeability estimator if the user is interested in the amount of chemical that is absorbed (ten Berge, 2010).

### **P\_DER2: Dermal Dose from Soil where Skin Contact with Soil, Dust, or Powder Occurs**

Dermal contact with residues of products applied to soils, such as soil amendments, and to powdered products such as powdered laundry detergent, may occur. For skin contact with chemicals in soil, the potential dermal dose is estimated by multiplying the chemical concentration in the soil (mass/mass) by an age-specific soil adherence factor describing the transfer of the chemical from the soil to the hands, fraction absorbed, and age-specific activity patterns to estimate potential loading on the skin ([Pawar et al. 2016](#)). For skin contact with powdered chemicals, the potential dermal dose is estimated by multiplying the chemical concentration in the product (mass/mass) by an age-specific adherence factor describing the transfer of the chemical from the powder to the hands, fraction absorbed, and age-specific activity patterns to estimate potential loading on the skin.

### **A\_DER1: Dermal Dose from Direct Transfer from Vapor Phase to Skin (Article Model)**

A\_INH1 model assumes emissions of semi-volatile organic compound (SVOC) additives from articles and subsequent partitioning between indoor air, airborne particles, and settled dust over time. 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 as estimated by A\_INH1 and the partitioning between air and skin lipids, which is 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](#)).

### **A\_DER2: Dermal Dose from Article where Skin Contact Occurs**

For articles that come into direct contact with the skin, chemical can migrate from the article to the skin. This is described by the migration rate to the skin, which is governed by the solid phase diffusion coefficient, in combination 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, for example mattresses versus toys ([Delmaar et al., 2013](#)).

### A\_DER3: Dermal Dose from Skin Contact with Dust

Dermal contact with chemicals in dust that settle on articles may occur. This model is similar to P\_DER2, for skin contact with chemicals in soil and powders. The potential dermal dose is estimated by multiplying the chemical concentration in the dust (mass/mass) by an age-specific soil adherence factor describing the transfer of the chemical from dust to the hands, fraction absorbed, and age-specific activity patterns to estimate potential loading on the skin ([Pawar et al. 2016](#)).

## 3. Detailed Descriptions of Models 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 E2 are determined in an alternate manner and are described in section E2.)

How a product's chemical emissions are represented in CEM depends on how the product is used and its chemical makeup. Emissions from each incidence of product usage 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. The 60-day modeling period for each incidence of usage was chosen after it was determined that airborne concentrations returned to background levels well within the 60-day window. This methodology allows for overlaying multiple 60-day windows, each associated with one incident of product usage to determine elevated concentrations associated with repeated use while maintaining rapid model run times. Sections E1 through E5 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 E2, A\_ING3, A\_ING1, and A\_DER1.

### Two-zone Mass Balance Model for Estimating Inhalation Exposure from Product Use

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 (E6). 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 2** and the equations for Zone 1 and Zone 2:

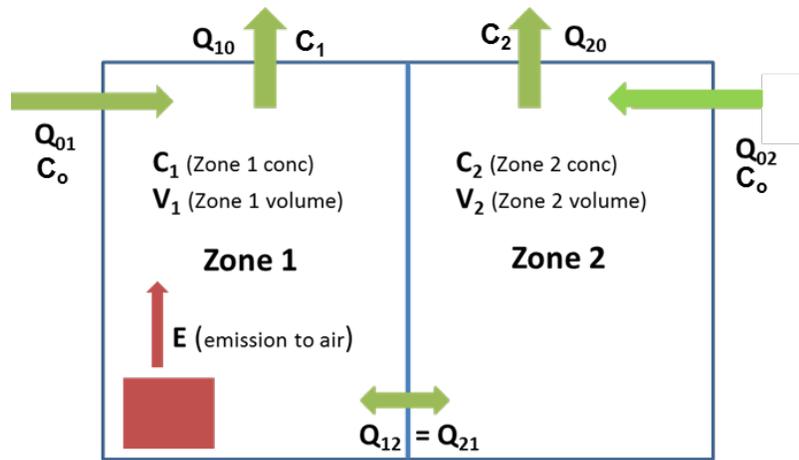


Figure 2. Schematic of two-zone model of indoor environment

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

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

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  $Q_{0x}/V_x$  ( $\text{hr}^{-1}$ )

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

$Q_{12}$  = Interzonal air flow rate ( $\text{m}^3/\text{hr}$ )

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

$V$  = Volume of Zone 1 or 2 ( $\text{m}^3$ )

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.

Air exchange rates and interzonal air flow are variables that can be edited. Default air exchange rates for the building are from the Exposure Factors Handbook ([U.S. EPA, 2011](#)). 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:

$$\text{Closed rooms: } Q_{12} = (0.078 + 0.31 \times AER) \times V \quad (3)$$

Open rooms:  $Q_{12} = (0.046 + 0.39 \times AER) \times V$  (4)

Where:

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

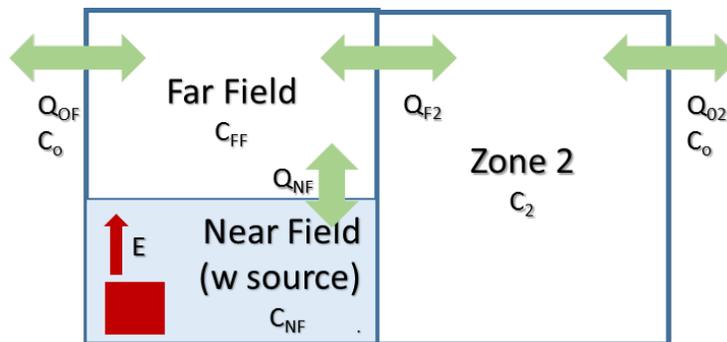
$V$  = Volume of building ( $m^3$ )

Default volumes for buildings and individual room sizes are taken from the Exposure Factors Handbook ([U.S. EPA, 2011](https://www.epa.gov/101/factors)). 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 20. This dilution factor was calculated using [Klepeis et al. \(2009\)](https://pubs.acs.org/doi/10.1021/ta02001a001) 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 Product 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 near-field option should be selected with care, generally only when a product user is stationary rather than mobile during the duration of product use. 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. The NFFF option can be selected on the Scenario tab for any product with an inhalation model.

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 3** and in the derivation of the governing differential equations.



**Figure 3. 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

$$\frac{dC_{NF}}{dt} = -AER_{NF} \times C_{NF} + AER_{NF} \times C_{FF} + \frac{E(t)}{V_{NF}} \quad (5)$$

#### Far Field, Zone 1

$$\frac{dC_{FF}}{dt} = -AER_{NF} \times C_{FF} \times \frac{V_{NF}}{V_{FF}} + AER_{NF} \times C_{NF} \times \frac{V_{NF}}{V_{FF}} + Q_{R1R2} \times \frac{C_{R2}}{V_{FF}} - AER_{R1} \times C_{FF} \times \frac{(V_{NF}+V_{FF})}{V_{FF}} - Q_{R1R2} \times \frac{C_{FF}}{V_{FF}} \quad (6)$$

#### Zone 2

$$\frac{dC_{R2}}{dt} = Q_{R1R2} \times \frac{C_{FF}}{V_{R2}} - AER_{R2} \times C_{R2} - Q_{R1R2} \times \frac{C_{R2}}{V_{R2}} \quad (7)$$

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 using an ordinary differential equation solver in Python, 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.

### E1: Emission from 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:

$$ER(t) = ER(0) \times e^{-kt} \quad (8)$$

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 ( $\text{min}^{-1}$ )

$t$  = 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 ( $VP$ ):

$$EvapTime = \frac{145}{(MW \times VP)^{0.9546}} \quad (9)$$

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

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

Users may also estimate  $k$  using another method shown in Equations 11 and 12,

$$k = \frac{E_0}{M_0} \quad (11)$$

$$E_0 = k_g \times C_{sat} \quad (\text{Error! Bookmark not defined.12})$$

Where,

$E_0$  = Emission factor ( $\mu\text{g}/\text{m}^2/\text{h}$ )

$k_g$  = Gas-phase mass transfer coefficient (m/h)

$C_{sat}$  = Saturation concentration based on the vapor pressure of chemical ( $\mu\text{g}/\text{m}^3$ )

$M_0$  = Mass of chemical per unit area ( $\mu\text{g}/\text{m}^2$ )

Where,

$$M_0 = \rho \times thickness \times CF_1 \times CF_2 \quad (13)$$

$\rho$  = Density of the chemical ( $\text{g}/\text{cm}^3$ )

$thickness$  = Thickness of the spill/puddle (assumed to be 0.01 cm)

$CF_1$  = Conversion factor,  $10^4 \text{ cm}^2/\text{m}^2$

$CF_2$  = Conversion factor,  $10^6 \mu\text{g}/\text{g}$

Typically Equations 11-13 are used when a user wants to model the emission from a chemical spill. When a user selects "Estimate All" on the Chemical Properties page, a dialogue box will appear that asks if you want to use the Emission Factor to calculate the decay rate. Selecting yes will then pop up another screen that asks if you want to estimate the

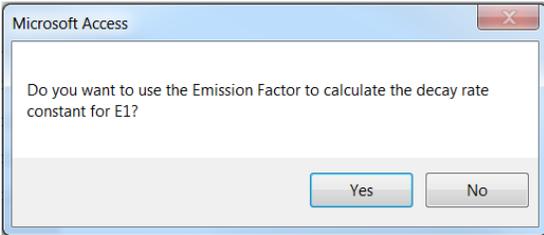
emission factor. If you want to use your own emission factor, select no and then manually enter the emission factor in the input box. If you do not want to use an emission factor, the emission factor input will be set to 0 and CEM will calculate  $k$  using Equation 10.

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: Ethylene glycol



$ER(0)$  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  $k$ .

$$ER(t) = \frac{M \times WF \times CF}{t_a} \times \left[ (1 - e^{-k(t-t_{start})}) - \left( (1 - e^{-k(t-(t_{start}+t_a))}) \times H(t) \right) \right] \quad (14)$$

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 ( $\text{min}^{-1}$ )
- $t$  = Time (min)
- $H(t)$  = 0/1 value used to indicate if product is actively in use
  - = 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.

Where:

$$M = Vol \times \rho \times Dil \times 10^6 \quad (15)$$

$M$	=	Mass of product used (g)
$Vol$	=	Volume of product (m <sup>3</sup> )
$\rho$	=	Product density (g/cm <sup>3</sup> )
$Dil$	=	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:

$$C_{sat} = \frac{((1.33 \times 10^5) \times VP \times MW)}{(R \times T)} \quad (16)$$

Where:

$C_{sat}$	=	Saturation concentration in air (µg/m <sup>3</sup> )
$VP$	=	Vapor pressure (torr)
$MW$	=	Molecular weight (g/mol)
$R$	=	Universal gas constant, 8.314 J/mol-K
$T$	=	Temperature (K)

For gases with very high vapor pressure, users should change the vapor pressure to be at atmospheric pressure when estimating  $C_{sat}$ . After clicking 'estimate' the user can edit the vapor pressure to be atmospheric pressure, which will be used to estimate  $C_{sat}$ . However, this will **not** change the vapor pressure entered in the CEM form on the chemical property input tab, as the vapor pressure is used in other calculations.

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).

## E2: Emission from 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).

$$ER_{1_1}(t) = \frac{M \times WF \times CF}{t_a} \times \left\{ \left[ f \times (1 - e^{-k_1(t-t_{start})}) + (1-f) \times (1 - e^{-k_2(t-t_{start})}) \right] - \left[ f \times (1 - e^{-k_1(t-(t_{start}+t_a))}) + (1-f) \times (1 - e^{-k_2(t-(t_{start}+t_a))}) \right] \times H(t) \right\} \quad (17)$$

Where:

- $ER_1(t)$  = 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)  
 $H(t)$  = 0/1 value used to indicate if product is actively in use  
= 0 if  $t - (t_{start} + t_a) < 0$   
= 1 if  $t - (t_{start} + t_a) > 0$   
 $k_1$  =  $233.25 \times (VP \div 24) \div 60$  ( $\text{min}^{-1}$ )  
 $k_2$  =  $0.0000584 \times (MW \div 24) \div 60$  ( $\text{min}^{-1}$ )  
 $VP$  = Vapor pressure (torr)  
 $MW$  = Molecular weight (g/mol)

$$ER_2(t) = \frac{M \times WF \times CF \times (1-f)}{t_a} \times \left[ (1 - e^{-k(t-t_{start})}) - \left( (1 - e^{-k(t-(t_{start}+t_a))}) \times H(t) \right) \right] \quad (18)$$

Where:

- $ER_2(t)$  = 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)  
 $f$  = Fraction of mass emitted from first exponential (0.1) (unitless)  
 $t_{start}$  = Time of start of application (min)  
 $t_a$  = Application time (min)  
 $k$  = First-order rate constant for emissions decline ( $\text{min}^{-1}$ )  
 $t$  = Time (min)

$$\begin{aligned}
H(t) &= 0/1 \text{ value used to indicate if product is actively in use} \\
&= 0 \text{ if } t - (t_{start} + t_a) < 0 \\
&= 1 \text{ if } t - (t_{start} + t_a) > 0
\end{aligned}$$

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 assumes a total of 25% mass released and 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 as shown in Equation 15.

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 E1 for further details.

### E3: Emission from Product Sprayed

The 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).

$$ER_1(t) = \frac{M \times WF \times CF \times f}{t_a} \times [1 - H(t)] \quad (19)$$

Where:

$$\begin{aligned}
ER_1(t) &= \text{Emission rate at time } t \text{ from initial aerosolized product (mg/min)} \\
M &= \text{Mass of product used (g)} \\
WF &= \text{Weight fraction of chemical in product (unitless)} \\
CF &= \text{Conversion factor (1000 mg/g)} \\
f &= \text{Fraction of product emitted to air (unitless)} \\
t_a &= \text{Application time (min)} \\
H(t) &= 0/1 \text{ value used to indicate if product is actively in use} \\
&= 0 \text{ if } t - (t_{start} + t_a) < 0 \\
&= 1 \text{ if } t - (t_{start} + t_a) > 0
\end{aligned}$$

$$ER_2(t) = \frac{M \times WF \times CF}{t_a} \times \left[ (1 - e^{-k(t-t_{start})}) - \left( (1 - e^{-k(t-(t_{start}+t_a))}) \times H(t) \right) \right] \quad (20)$$

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 ( $\text{min}^{-1}$ )

$t$  = Time (min)

$H(t)$  = 0/1 value used to indicate if product is actively in use

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

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

$$ER_{final}(t) = ER_1(t) + ER_2(t) \quad (21)$$

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 as shown in Equation 15.

At each time step CEM checks whether the current value for the emission rate results in an indoor concentration that exceeds  $C_{sat}$ . If so, then the emission rate is reduced to a value that results in the indoor concentration equaling  $C_{sat}$ . See E1 for further details.

#### E4: Emission from Product Added to Water

The 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.

$$EvapTime = \frac{145}{(MW \times VP)^{0.9546}} \times 60 \quad (22)$$

Where:

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

$$ER(t) = \frac{M \times WF \times CF}{EvapTime} \times H(t) \quad (23)$$

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)  
 $H(t)$  = 0/1 value used to indicate if product is actively in use  
           = 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 as shown in Equation 15.

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 E1 for further details.

## E5: Emission from Product Placed in Environment

The model assumes emission at a constant rate over a duration that depends on its molecular weight and vapor pressure, as shown in Equations 22 and 23. 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.

The mass of product used ( $M$ ) can be specified directly or estimated from the volume of product used, product density, and product dilution as shown in Equation 15.

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 E1 for further details.

## P\_INH1 and P\_INH2: Calculation of Inhalation Dose from Product Usage

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

$$LADC = \frac{C_{ati} \times FQ \times ED}{AT \times CF_1} \quad (24)$$

Where:

- $LADC$  = Potential Lifetime Average Daily Concentration (mg/m<sup>3</sup>-day)
- $C_{ati}$  = Time-integrated air concentration for an event (mg/m<sup>3</sup>-event)
- $FQ$  = Frequency of product use (events/year)
- $ED$  = Exposure duration (years of product usage)
- $AT$  = Averaging time (years), assumed to an entire lifetime (78 years) for LADC
- $CF_1$  = Conversion factor (365 days/year)

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

$$C_{ati} = \sum_{ST}^{ET} C_{i,t} \times \Delta t \quad (25)$$

Where:

- $C_{ati}$  = Time-integrated, air concentration for an event (mg/m<sup>3</sup>-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/m<sup>3</sup>)
- $\Delta t$  = time interval (3.47 x 10<sup>-4</sup> 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.

$$C_p = \text{Max}[[C_{i,t}]_{ST}^{ET}] \quad (26)$$

Where:

- $C_p$  = Potential Peak Concentration (mg/m<sup>3</sup>), evaluated as the maximum  $C_{i,t}$  from t=0 to t=ET
- $C_{i,t}$  = Concentration in Zone i at time t (mg/m<sup>3</sup>)

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:

$$CADD = \frac{C_{air} \times Inh \times FQ \times D \times ED}{BW \times AT \times CF_1} \quad (27)$$

Where:

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

*C<sub>air</sub>* = Concentration of chemical in air (mg/m<sup>3</sup>)

*Inh* = Inhalation rate (m<sup>3</sup>/hr)

*FQ* = Frequency of use (events/year)

*D* = Duration of use (hr/event)

*ED* = Exposure duration (years of product usage)

*BW* = Body weight (kg)

*AT* = Averaging time (years)

*CF<sub>1</sub>* = Conversion factor (365 days/year)

CEM uses two different inhalation rates, one when the receptor is using the product and another after the use has ended. **Table 2** shows the inhalation rates by receptor age category for during and after product use.

**Table 2. Inhalation rates used in CEM product models.**

Receptor category	Inhalation Rate During Use (m <sup>3</sup> /hr) <sup>a</sup>	Inhalation Rate After Use (m <sup>3</sup> /hr) <sup>b</sup>
Adult (≥21 years)	0.74	0.61
Youth (16-20 years)	0.72	0.68
Youth (11-15 years)	0.78	0.63
Child (6-10 years)	0.66	0.5
Small Child (3-5 years)	0.66	0.42
Infant (1-2 years)	0.72	0.35
Infant (<1 year)	0.46	0.23

<sup>a</sup>Table 6-2, light intensity values (EPA, 2011)

<sup>b</sup>Table 6-1 (EPA, 2011)

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, CADD is calculated using the following expression:

$$CADD = \frac{Dose_{ati} \times FQ \times ED}{BW \times AT \times CF_1} \quad (28)$$

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 1 year. In turn, the time-integrated air dose is calculated as follows:

$$Dose_{ati} = \sum_{ST}^{ET} C_{i,t} \times \Delta t \times Inh_{i,t} \times CF_2 \quad (29)$$

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/m<sup>3</sup>)
- $Inh_{i,t}$  = Inhalation Rate for Zone i at time t (m<sup>3</sup>/hr)
- $\Delta t$  = Time interval (1.16 x 10<sup>-4</sup> 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 Lifetime Average Daily Dose (LADD) represents chronic exposures over a lifetime and can also be calculated in CEM. Users can calculate the LADD by changing the chronic exposure duration to a value for the specific product or article of interest and change the chronic averaging time to the 78 years (an entire lifetime). The LADD should be used for adult only.

The LADD uses an averaging time of a lifetime, which is typically 78 years. Suggested LADD exposure durations for products used regularly are 57 years, for products used intermittently are 12 years, and for those used less often are 5 years. The suggested exposure durations were based on an exposure starting at 21 years old and continuing each year of an adult's lifetime (78-21 = 57), an exposure starting at 18 years old and occurring every 5 years (78-18 = 60/5 = 12), and an exposure occurring for only 5 years throughout a lifetime. Note, articles can generally be assumed to have a continuous exposure duration in that exposure duration and averaging time are likely to match.

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

$$ADR = \frac{C_{air} \times Inh \times FQ \times D \times ED}{BW \times AT} \quad (30)$$

Where:

- ADR* = Potential Acute Dose Rate (mg/kg-day)  
*C<sub>air</sub>* = Concentration of chemical in air (mg/m<sup>3</sup>)  
*Inh* = Inhalation rate (m<sup>3</sup>/hr)  
*FQ* = Frequency of product use (events/day)  
*D* = Duration of use (hr/event)  
*ED* = Exposure duration (days of product usage)  
*BW* = Body weight (kg)  
*AT* = Averaging time (days)

For the ADR calculations, an averaging time of 1 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<sub>ati</sub> is used:

$$Dose_{ati} = \sum_{ST}^{ET} C_{i,t} \times \Delta t \times Inh_{i,t} \times CF_2 \quad (31)$$

Where:

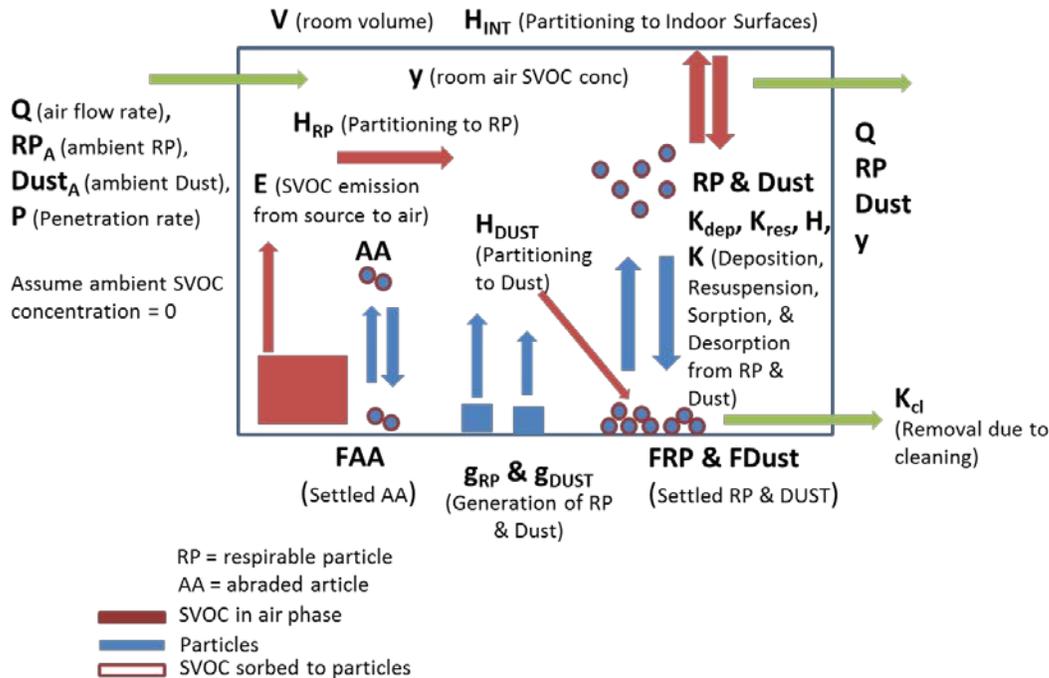
- Dose<sub>ati</sub>* = Time-integrated, air dose for an event (mg/event) from start time (ST) to end time (ET), where ET = ST + 60 days.  
*C<sub>i,t</sub>* = Concentration in Zone i at time t (mg/m<sup>3</sup>)  
*Inh<sub>i,t</sub>* = Inhalation Rate for Zone i at time t (m<sup>3</sup>/hr)  
 $\Delta t$  = Time interval (1.16 x 10<sup>-4</sup> days/event)  
*CF<sub>2</sub>* = 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 airborne 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.

## E6: Emission from Article Placed in Environment

The mechanisms that control SVOC behavior in an indoor environment are shown in Figure 4. These include SVOC emissions, article abrasion, 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 4. 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, 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 respirable particles, “RP”).
- 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.
- Abrasion of the emitting article is modeled as a first order physical decay process. Abrasion is assumed not to change the area of the emitting surface; as a result, the article’s physical mass balance is not maintained. Provided the abrasion rate is low, as may be reasonably expected, this assumption is a justifiable simplification. Chemical mass balance is strictly preserved, however, in all respects.
- Abraded particles are distinct from dust and respirable particles and constitute a third particle species in the model. Abraded particles are first emitted to the air and thereafter may deposit on and resuspend from the floor; like other particulates in the model, these particles are subject to cleaning and ventilation losses. Abraded particles, 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. Abraded particles settled on the floor are assumed to have a hemispherical area available for emission, whereas those suspended in the air have a spherical area available for emission.

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  $\mu\text{m}$ ), 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, by either 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 3 itemizes the chemical and physical parameters and their representational symbols that feature in the set of 10 differential equations that define the model.

**Table 3. Physical-Chemical Parameters Referenced in Model Equations**

Symbol	Property	Units
<i>Physical Parameters</i>		
V	Volume of the room	$\text{m}^3$
Q	Ventilation rate of the room	$\text{m}^3/\text{hr}$
As	Area of emitting article surface	$\text{m}^2$

Symbol	Property	Units
$L_{Art}$	Thickness of emitting article surface	m
$\rho_{Art}$	Density of emitting article	mg / m <sup>3</sup>
$k_{depTSP}$	TSP deposition rate constant	1/hr
$k_{depDust}$	Dust deposition rate constant	1/hr
$k_{depAbArt}$	Abraded article particle deposition rate constant	1/hr
$k_{reSTSP}$	TSP resuspension rate constant	1/hr
$k_{reSDust}$	Dust resuspension rate constant	1/hr
$k_{reSAbArt}$	Abraded article particle resuspension rate constant	1/hr
$g_{abr}$	Mass generation rate of abraded article particles	mg/hr
$g_{ATSP}$	Mass generation rate of TSP into indoor air	mg/hr
$g_{ADust}$	Mass generation rate of dust into indoor air	mg/hr
$g_{FTSP}$	Mass generation rate of TSP onto indoor floor	mg/hr
$g_{FDust}$	Mass generation rate of dust onto indoor floor	mg/hr
$AmbTSPConc$	Concentration of TSP in ambient air	mg/m <sup>3</sup>
FilterPen	Air Filter Penetration Ratio	None
Clpr	Cleaning Periodicity	/hr
cleff	Cleaning Efficiency	None
$k_{ci}(t)$	Binary switch representing whether cleaning is ongoing (based on Clpr)	None
$Z(t)$	Binary switch representing whether product is present in room	None
$\rho_{TSP}$	Density of TSP particle	mg/m <sup>3</sup>
$\rho_{Dust}$	Density of dust particle	mg/m <sup>3</sup>
$r_{TSP}$	Radius of TSP particle	m
$r_{Dust}$	Radius of dust particle	m
$r_{AbArt}$	Radius of abraded article particles	m
$A_{Int}$	Area of interior surfaces	m <sup>2</sup>
$L_{Int}$	Thickness of sorbing portion of interior surfaces	m
<b>Chemical Parameters</b>		
h	SVOC gas phase mass transfer coefficient	m/hr
$K_{TSP}$	SVOC TSP-air partition coefficient	m <sup>3</sup> /mg
$K_{Dust}$	SVOC dust-air partition coefficient	m <sup>3</sup> /mg
$K_{Art}$	SVOC article-air partition coefficient	None
$K_{Int}$	SVOC -air partition coefficient	None
$H_{TSP}$	TSP overall gas-phase mass transfer coefficient	m/hr
$H_{Dust}$	Dust overall gas-phase mass transfer coefficient	m/hr
$H_{Int}$	Interior surfaces overall gas-phase mass transfer coefficient	m/hr
$H_{AbArt}$	Abraded article particle overall gas-phase mass transfer coefficient	m/hr
$C_{0Art}$	Initial concentration of SVOC in emitting article	µg/m <sup>3</sup>
<b>Inventory Terms</b>		
$N_{air}$	SVOC mass in the gas phase in air	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
$N_{A\_AbArt}$	Air (suspended) abraded article SVOC mass	µg
$N_{F\_AbArt}$	Floor (settled) abraded article SVOC mass	µg
$A_{TSP}$	Mass of TSP suspended in the air	mg
$A_{Dust}$	Mass of dust suspended in the air	mg
$A_{AbArt}$	Mass of abraded article suspended in the air	mg
$F_{TSP}$	Mass of TSP settled on the floor	mg
$F_{Dust}$	Mass of dust settled on the floor	mg
$F_{AbArt}$	Mass of abraded article settled on the floor	mg

<sup>a</sup>The thickness of emitting article surface value can impact emissions. EPA is considering article-specific thicknesses.

Default model inputs are provided in Table B-12. A description of inputs that are estimated via physical-chemical properties is presented in the following section. The area of interior surfaces is estimated using the following equation from EPA's Exposure Factors Handbook ([U.S. EPA, 2011](#)).

$$A_{int} = 2.08 \times V \quad (32)$$

Where:

$A_{int}$  = Area of Interior Surfaces (m<sup>2</sup>)

$V$  = Volume of Room (m<sup>3</sup>)

### *Model Equations*

The following set of 14 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 using an ordinary differential equation solver in Python, the model is able to produce time-varying estimates of SVOC mass in various media as well as dust and RP mass in air and on the floor. Cleaning periodicity, or the frequency that cleaning is conducted, is incorporated as a switch and is not shown explicitly in the equations below. That is, if cleaning is conducted weekly, at a given time-step each week, mass of settled chemical will be removed, as governed by the cleaning efficiency and mass of settled particles.

### **Mass Balance for SVOC in Gas Phase**

$$\begin{aligned}
\frac{dN_{Air}}{dt} = & Z(t) \times h \times A_s \times \frac{C_{0Art}}{K_{Art}} \times e^{-\left(\frac{h}{K_{Art} \times L_{Art}} \times t\right)} \\
& - \frac{Q}{V} \times N_{air} \\
& - H_{TSP} \times \frac{A_{TSP}}{\rho_{TSP}} \times \frac{3}{r_{TSP}} \times \left( \frac{N_{air}}{V} - \frac{N_{ATSP}}{A_{TSP}} \times \frac{1.0}{K_{TSP}} \right) \\
& - H_{Dust} \times \frac{A_{Dust}}{\rho_{Dust}} \times \frac{3}{r_{Dust}} \times \left( \frac{N_{air}}{V} - \frac{N_{ADust}}{A_{Dust}} \times \frac{1.0}{K_{Dust}} \right) \\
& - H_{TSP} \times \frac{F_{TSP}}{\rho_{TSP}} \times \frac{1.5}{r_{TSP}} \times \left( \frac{N_{air}}{V} - \frac{N_{FTSP}}{F_{TSP}} \times \frac{1.0}{K_{TSP}} \right) \\
& - H_{Dust} \times \frac{F_{Dust}}{\rho_{Dust}} \times \frac{1.5}{r_{Dust}} \times \left( \frac{N_{air}}{V} - \frac{N_{FDust}}{F_{Dust}} \times \frac{1.0}{K_{Dust}} \right) \\
& - H_{Int} \times \left( \frac{N_{air}}{V} - \frac{N_{Int}}{A_{Int} \times L_{Int}} \times \frac{1.0}{K_{Int}} \right) \times A_{Int} \\
& - H_{AbArt} \times \frac{A_{AbArt}}{\rho_{Art}} \times \frac{3}{r_{AbArt}} \times \left( \frac{N_{air}}{V} - \frac{N_{A\_AbArt}}{A_{AbArt}} \times \frac{\rho_{Art}}{K_{Art}} \right) \\
& - H_{AbArt} \times \frac{F_{AbArt}}{\rho_{Art}} \times \frac{1.5}{r_{AbArt}} \times \left( \frac{N_{air}}{V} - \frac{N_{F\_AbArt}}{F_{AbArt}} \times \frac{\rho_{Art}}{K_{Art}} \right)
\end{aligned} \tag{33}$$

#### Mass Balance for SVOC Sorbed to Suspended RP

$$\begin{aligned}
\frac{dN_{ARP}}{dt} = & H_{RP} \times \frac{A_{RP}}{\rho_{RP}} \times \frac{3}{r_{RP}} \times \left( \frac{N_{air}}{V} - \frac{N_{ARP}}{A_{RP}} \times \frac{1.0}{K_{RP}} \right) \\
& + kres_{RP} \times N_{FRP} - kdep_{RP} \times N_{ARP} - \frac{Q}{V} \times N_{ARP}
\end{aligned} \tag{34}$$

#### Mass Balance for SVOC Sorbed to Suspended Dust

$$\begin{aligned}
\frac{dN_{ADust}}{dt} = & H_{Dust} \times \frac{A_{Dust}}{\rho_{Dust}} \times \frac{3}{r_{Dust}} \times \left( \frac{N_{air}}{V} - \frac{N_{ADust}}{A_{Dust}} \times \frac{1.0}{K_{Dust}} \right) \\
& + kres_{Dust} \times N_{FDust} - kdep_{Dust} \times N_{ADust} - \frac{Q}{V} \times N_{ADust}
\end{aligned} \tag{35}$$

#### Mass Balance for SVOC Sorbed to Settled RP

$$\begin{aligned}
\frac{dN_{FRP}}{dt} = & H_{RP} \times \frac{F_{RP}}{\rho_{RP}} \times \frac{1.5}{r_{TR}} \times \left( \frac{N_{air}}{V} - \frac{N_{FRP}}{F_{RP}} \times \frac{1.0}{K_{RP}} \right) \\
& - kres_{RP} \times N_{FRP} + kdep_{RP} \times N_{ARP} - k_{cl}(t) \times Cl_{eff} \times N_{FRP}
\end{aligned} \tag{36}$$

### Mass Balance for SVOC Sorbed to Settled Dust

$$\begin{aligned} \frac{dN_{FDust}}{dt} = & H_{Dust} \times \frac{F_{Dust}}{\rho_{Dust}} \times \frac{1.5}{r_{Dust}} \times \left( \frac{N_{air}}{V} - \frac{N_{FDust}}{F_{Dust}} \times \frac{1.0}{K_{Dust}} \right) \\ & - kres_{Dust} \times N_{FDust} + kdep_{Dust} \times N_{ADust} - k_{cl}(t) \times Cl_{eff} \times N_{FTSP} \end{aligned} \quad (37)$$

### Mass Balance for SVOC Sorbed to Interior Surfaces (Sinks)

$$\frac{dN_{int}}{dt} = H_{Int} \times \left( \frac{N_{air}}{V} - \frac{N_{Int}}{A_{Int} \times L_{Int}} \times \frac{1.0}{K_{Int}} \right) \times A_{Int} \quad (38)$$

### Mass Balance for Suspended RP

$$\frac{dA_{RP}}{dt} = g_{ARP} + Q \times AmbRPConc \times FilterPen - \frac{Q}{V} \times A_{RP} - kdep_{RP} \times A_{RP} + kres_{RP} \times F_{RP} \quad (39)$$

### Mass Balance for Suspended Dust

$$\frac{dA_{Dust}}{dt} = g_{ADust} - \frac{Q}{V} \times A_{Dust} - kdep_{Dust} \times A_{Dust} + kres_{Dust} \times F_{TSP} \quad (40)$$

### Mass Balance for Settled RP

$$\frac{dF_{RP}}{dt} = g_{FRP} + kdep_{RP} \times A_{RP} - kres_{RP} \times F_{RP} - k_{cl}(t) \times Cl_{eff} \times F_{RP} \quad (41)$$

### Mass Balance for Settled Dust

$$\frac{dF_{dust}}{dt} = g_{FDust} + kdep_{Dust} \times A_{Dust} - kres_{Dust} \times F_{Dust} - k_{cl}(t) \times Cl_{eff} \times F_{Dust} \quad (42)$$

### Mass Balance for SVOC in Suspended Abraded Article Particles

$$\begin{aligned} \frac{dN_{A\_AbArt}}{dt} = & g_{abr} \div \rho_{Art} \times C_{0Art} \times e^{-\left(\frac{h}{K_{Art} \times L_{Art}} \times x\right)} \\ & + H_{AbArt} \times \frac{A_{AbArt}}{\rho_{Art}} \times \frac{3}{r_{AbArt}} \times \left( \frac{N_{air}}{V} - \frac{N_{A\_AbArt}}{A_{AbArt}} \times \frac{\rho_{Art}}{K_{Art}} \right) \\ & + kres_{AbArt} \times N_{F\_AbArt} \\ & - kdep_{AbArt} \times N_{A\_AbArt} \\ & - \frac{Q}{V} \times N_{A\_AbArt} \end{aligned} \quad (43)$$

### Mass Balance for SVOC in Settled Abraded Article Particles

$$\begin{aligned}
\frac{dN_{F\_AbArt}}{dt} = & +H_{AbArt} \times \frac{F_{AbArt}}{\rho_{Art}} \times \frac{1.5}{r_{AbArt}} \times \left( \frac{N_{air}}{V} - \frac{N_{F\_AbArt}}{F_{AbArt}} \times \frac{\rho_{Art}}{K_{Art}} \right) \\
& - kres_{AbArt} \times N_{F\_AbArt} \\
& + kdep_{AbArt} \times N_{A\_AbArt} \\
& - k_{cl}(t) \times Cl_{eff} \times N_{F\_AbArt}
\end{aligned} \tag{44}$$

### Mass Balance for Suspended Abraded Article Particles

$$\begin{aligned}
\frac{dA_{AbArt}}{dt} = & g_{abr} \\
& + kres_{AbArt} \times F_{AbArt} \\
& - kdep_{AbArt} \times A_{AbArt} \\
& - \frac{Q}{V} \times A_{AbArt}
\end{aligned} \tag{45}$$

### Mass Balance for Settled Abraded Article Particles

$$\begin{aligned}
\frac{dF_{AbArt}}{dt} = & -kres_{AbArt} \times F_{AbArt} \\
& + kdep_{AbArt} \times A_{AbArt} \\
& - k_{cl}(t) \times Cl_{eff} \times F_{AbArt}
\end{aligned} \tag{46}$$

Note: In Equations 34, 35, and 43, the value of  $3/r$  is used to describe the surface area to volume ratio of a sphere. In Equations 36, 37, and 44, the value of  $1.5/r$  indicates that for settled particles, only half of the surface area is available for mass transfer.

### Estimation of Chemical Parameters from Basic Physical-Chemical Properties

As noted in Table 3, 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, 1990) 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:

$$h = 46.8 \times \frac{3.3}{(2.5 + MW^{1/3})^2} \tag{47}$$

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. We selected this simple empirical model (Equation 47) to create the default value and, at the same time, give the users the option of entering their own value by using external models.

#### Estimating $K_{RP}$ and $K_{Dust}$

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

$$K_p = f_{om\_part} \times \frac{K_{oa}}{\rho_{part}} \quad (48)$$

Where:

$K_p$  = SVOC partition coefficient for RP ( $K_{RP}$ ) or dust ( $K_{Dust}$ ) (m<sup>3</sup>/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)

$\rho_{part}$  = density of airborne particles; suggested value  $1 \times 10^9$  (mg/m<sup>3</sup>)

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.

We recommend estimating the particle-air partitioning coefficient based on the octanol-air partition coefficient ( $K_{oa}$ ) rather than vapor pressure for the following reasons: (1) While several empirical models are available for estimating the particle-air partitioning coefficients of VOCs based on their vapor pressure, few are available for SVOCs. (2) Unlike VOCs, the vapor pressures for SVOCs are difficult to determine experimentally at normal temperature. Consequently, there is a dearth of reliable vapor pressure data for SVOCs at normal temperature. (3) The octanol-air partition coefficient ( $K_{oa}$ ) for both VOCs and SVOCs can be determined either experimentally or from QSAR models. Currently, at least three QSAR models are available for estimating  $K_{oa}$  (Fu et al., 2016).

#### 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](#)):

$$\ln(K_{solid}) = 8.86 - 0.785 \times \ln(V_p) \quad (49)$$

Where:

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

$V_p$  = the vapor pressure of the SVOC (Torr)

#### Estimating $H_{Int}$ , $H_{Dust}$ , $H_{RP}$ and $H_{AbArt}$

$$D_s = \frac{3 \times 10^{-10}}{(MW + 292)^{0.65}} \quad (50)$$

Where:

$D_s$  = Solid-phase diffusion coefficient (m<sup>2</sup>/hr)

$MW$  = Molecular weight (g/mol)

$$K_{solid} = e^{(8.86-0.785 \times \ln(VP))} \quad (51)$$

Where:

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

$VP$  = Vapor pressure (torr)

$$h_a = 46.8 \times (3.3 \div (2.5 + MW^{\frac{1}{3}}))^2 \quad (52)$$

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 RP) and the air can be estimated based on the following relationship, where 'solid' refers to Int, RP, or Dust as appropriate ([U.S. EPA, 2005](#)):

$$\frac{1}{H_{solid}} = \frac{1}{h_a} + \frac{1}{\frac{2D_s}{L}K_{solid}} \quad (53)$$

Where:

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

$h_a$  = the SVOC gas phase mass transfer coefficient (m/hr), which is estimated earlier in equation (52)

$D_s$  = the SVOC solid-phase diffusion coefficient ( $m^2/hr$ )

$L$  = 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:

$$\left(\frac{D_0}{D_1}\right) = \left(\frac{MW_1}{MW_0}\right)^{0.65} \quad (54)$$

Where:

$D_0$  =  $3 \times 10^{-11}$  ( $m^2/h$ ) is the diffusion coefficient for the reference compound (PCB-52)

$D_1$  = diffusion coefficient for compound of interest ( $m^2/h$ )

$MW_0$  = 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 0.005 m 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.

## A\_INH1: 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 RP-bound SVOCs are assumed to be available for inhalation. The general expression for the Potential Chronic Average Daily Dose (CADD) is as follows:

$$CADD_{Air} = \frac{C_{gas\_avg} \times FracTime \times InhalAfter \times CF_1}{BW \times CF_2} \quad (55)$$

$$CADD_{Particulate} = \frac{SVOCRP_{air\_avg} \times RP_{air\_avg} \times (1 - IF_{RP}) \times FracTime \times InhalAfter \times CF_1}{BW \times CF_2} \quad (56)$$

$$CADD_{total} = CADD_{Air} + CADD_{Particulate} \quad (57)$$

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 ( $\mu\text{g}/\text{m}^3$ )
$SVOCRP_{air\_avg}$	=	Average SVOC in RP concentration, air ( $\mu\text{g}/\text{mg}$ )
$RP_{air\_avg}$	=	Average RP concentration, air ( $\text{mg}/\text{m}^3$ )
$IF_{RP}$	=	RP ingestion fraction (unitless)
$FracTime$	=	Fraction of time in environment (unitless)
$InhalAfter$	=	Inhalation rate after use ( $\text{m}^3/\text{hr}$ )
$CF_1$	=	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:

$$ADR_{Air} = \frac{C_{gas\_max} \times FracTime \times InhalAfter \times CF_1}{BW \times CF_2} \quad (58)$$

$$ADR_{Particulate} = \frac{SVOCRP_{air\_max} \times RP_{air\_avg} \times FracTime \times InhalAfter \times CF_1}{BW \times CF_2} \quad (59)$$

$$ADR_{total} = ADR_{Air} + ADR_{Particulate} \quad (60)$$

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 ( $\mu\text{g}/\text{m}^3$ )
$SVOCRP_{air\_max}$	=	Maximum SVOC in RP concentration, air ( $\mu\text{g}/\text{mg}$ )
$RP_{air\_max}$	=	Maximum RP concentration, air ( $\text{mg}/\text{m}^3$ )
$FracTime$	=	Fraction of time in environment (unitless)
$InhalAfter$	=	Inhalation rate after use ( $\text{m}^3/\text{hr}$ )
$CF_1$	=	Conversion factor (24 hrs/day)
$BW$	=	Body weight (kg)
$CF_2$	=	Conversion factor (1000 $\mu\text{g}/\text{mg}$ )

## P\_ING1: Ingestion of Product Swallowed

The 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](#)).

$$CADD = \frac{FQ_{cr} \times M \times WF \times F_{ing} \times CF_1 \times ED_{cr}}{BW \times AT_{cr} \times CF_2} \quad (61)$$

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), 78 years for LADD
$BW$	=	Body weight (kg)
$CF_1$	=	Conversion factor (1000 mg/g)
$CF_2$	=	Conversion factor (365 days/year)

$$ADR = \frac{FQ_{ac} \times M \times WF \times F_{ing} \times CF_1 \times ED_{ac}}{BW \times AT_{ac}} \quad (62)$$

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)

## P\_ING2: Ingestion of Product Applied to Ground Outdoors

The 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. As currently incorporated, the CADD reports the average dose over one year, resulting in the value of 365 multiplied by the natural log of 2, in the half-life terms of the equation. This is multiplied by the soil ingestion rate, exposure duration, averaging time, and body weight to calculate dose ([U.S. EPA, 2012b](#)).

$$CADD = \frac{M \times WF \times Freq \times D \times \left( \frac{1}{\frac{365 \ln(2)}{t_{1/2}}} \right) \times \left( 1 - e^{-\left( \frac{365 \ln(2)}{t_{1/2}} \right)} \right) \times SoilIng \times ED_{cr} \times CF_1}{Area \times Depth \times \rho \times (1 - \phi) \times AT_{cr} \times BW} \quad (63)$$

Where:

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

- SoilIng* = Incidental soil ingestion rate (mg/day)
- ED<sub>cr</sub>* = Exposure duration, chronic (years)
- CF<sub>1</sub>* = Conversion factor (1 kg/1000 g)
- Area* = Area of yard product is applied (m<sup>2</sup>)
- Depth* = Mixing depth of soil (m)
- ρ* = Soil density (kg/m<sup>3</sup>)
- ∅* = Soil porosity (unitless)
- AT<sub>cr</sub>* = Averaging time, chronic (years), 78 years for lifetime
- BW* = Body weight (kg)

$$ADR = \frac{M \times WF \times SoilIng \times ED_{ac} \times CF_1}{Area \times Depth \times \rho \times (1 - \emptyset) \times AT_{ac} \times BW} \quad (64)$$

Where:

- ADR* = Potential Acute Dose Rate (mg/kg-day)
- M* = Mass of product used (g)
- WF* = Weight fraction of chemical in product (unitless)
- SoilIng* = Incidental soil ingestion rate (mg/day)
- CF<sub>1</sub>* = Conversion factor (1 kg/1000 g)
- ED<sub>ac</sub>* = Exposure duration, acute (days)
- Area* = Area of yard product is applied (m<sup>2</sup>)
- Depth* = Mixing depth of soil (m)
- ρ* = Soil density (kg/m<sup>3</sup>)
- ∅* = Soil porosity (unitless)
- AT<sub>ac</sub>* = Averaging time, acute (days)
- BW* = Body weight (kg)

Users may enter the chemical half-life in CEM, if known. If unknown, ECHA provides the following guidance in Table **Table 4** based on *K<sub>p</sub>*, soil and standard biodegradation test results (ECHA, 2016). For *K<sub>p</sub>* values above 10,000, the half-life scales according to the pattern listed in the table.

**Table 4. Chemical half-life in soil (in days).**

<i>K<sub>p</sub></i> , soil	Readily biodegradable	Readily biodegradable, failing 10-d window	Inherently biodegradable
<100	30	90	300
>100, <1000	300	900	3,000

Kp, soil	Readily biodegradable	Readily biodegradable, failing 10-d window	Inherently biodegradable
>1000, <10,000	3,000	9,000	30,000

## A\_ING1: Ingestion after Inhalation (Article Model)

The Article Model described in E6 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 (RP) and large particles (Dust) that will be inhaled and trapped in the upper airway. The fraction that is trapped in the airway is termed the ingestion fraction (IF). The mass trapped is assumed to be available for ingestion.

$$CADD_{IAI} = \frac{(SVO CRP_{air\_avg} \times RP_{air\_avg} \times IF_{RP} + SVO CDust_{air\_avg} \times Dust_{air\_avg} \times IF_{Dust}) \times InhalAfter \times CF_1}{BW \times CF_2} \quad (65)$$

Where:

$CADD_{IAI}$  = Potential Chronic Average Daily Dose from ingestion after inhalation (mg/kg-day)

$SVO CRP_{air\_avg}$  = Average SVOC in RP concentration, air ( $\mu\text{g}/\text{mg}$ )

$RP_{air\_avg}$  = Average RP concentration, air ( $\text{mg}/\text{m}^3$ )

$IF_{RP}$  = RP ingestion fraction (unitless)

$SVO CDust_{air\_avg}$  = Average SVOC dust concentration, air ( $\mu\text{g}/\text{mg}$ )

$Dust_{air\_avg}$  = Average dust concentration, air ( $\text{mg}/\text{m}^3$ )

$IF_{Dust}$  = Dust ingestion fraction (unitless)

$InhalAfter$  = Inhalation rate after use ( $\text{m}^3/\text{hr}$ )

$CF_1$  = Conversion factor (24 hrs/day)

$BW$  = Body weight (kg)

$CF_2$  = Conversion factor (1000 mg/g)

$$ADR_{IAI} = \frac{(SVO CRP_{air\_max} \times RP_{air\_max} \times IF_{TSP} + SVO CDust_{air\_max} \times Dust_{air\_max} \times IF_{Dust}) \times InhalAfter \times CF_1}{BW \times CF_2} \quad (66)$$

Where:

$ADR_{IAI}$  = Potential Acute Dose Rate from Ingestion and Inhalation (mg/kg-day)

$SVO CRP_{air\_max}$  = Maximum SVOC in RP concentration, air ( $\mu\text{g}/\text{mg}$ )

$RP_{air\_max}$  = Maximum RP concentration, air ( $\text{mg}/\text{m}^3$ )

$IF_{TSP}$  = RP ingestion fraction (unitless)

$SVO CDust_{air\_max}$  = Maximum SVOC in dust concentration, air ( $\mu\text{g}/\text{mg}$ )

$Dust_{air\_max}$	= Maximum dust concentration, air (mg/m <sup>3</sup> )
$IF_{Dust}$	= Dust ingestion fraction (unitless)
$InhalAfter$	= Inhalation rate after use (m <sup>3</sup> /hr)
$CF_1$	= Conversion factor (24 hrs/day)
$BW$	= Body weight (kg)
$CF_2$	= Conversion factor (1000 mg/g)

## A\_ING2: Ingestion of Article Mouthed (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](#)).

$$CADD = \frac{MR \times CA \times D \times ED_{cr} \times CF_1}{BW \times AT_{cr} \times CF_2} \quad (67)$$

Where:

$CADD$	= Potential Chronic Average Daily Dose (mg/kg-day)
$MR$	= Migration rate of chemical from article to saliva (mg/cm <sup>2</sup> /hr)
$CA$	= Contact area of mouthing (cm <sup>2</sup> )
$D$	= Duration of mouthing (min/hr)
$ED_{cr}$	= Exposure duration, chronic (years)
$AT_{cr}$	= Averaging time, chronic (years)
$BW$	= Body weight (kg)
$CF_1$	= Conversion factor (24 hrs/day)
$CF_2$	= Conversion factor (60 min/hr)

$$ADR = \frac{MR \times CA \times D \times ED_{ac} \times CF_1}{BW \times AT_{ac} \times CF_2} \quad (68)$$

Where:

$ADR$	= Potential Acute Dose Rate (mg/kg-day)
$MR$	= Migration rate of chemical from article to saliva (mg/cm <sup>2</sup> /hr)
$CA$	= Contact area of mouthing (cm <sup>2</sup> )
$D$	= Duration of mouthing (min/hr)
$ED_{ac}$	= Exposure duration, acute (days)

- $AT_{ac}$  = Averaging time, acute (days)  
 $BW$  = Body weight (kg)  
 $CF_1$  = Conversion factor (24 hrs/day)  
 $CF_2$  = Conversion factor (60 min/hr)

### A\_ING3: Incidental Dust Ingestion (Article Model)

The Article Model described in E6 calculates SVOC concentration in small particles (termed RP) 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.

$$CADD = \frac{(SVOCRP_{floor\_avg} + SVOCDust_{floor\_avg}) \times FracTime \times DustIng}{BW \times CF} \quad (69)$$

Where:

- $CADD$  = Potential Chronic Average Daily Dose (mg/kg-day)  
 $SVOCRP_{floor\_avg}$  = Average SVOC in RP concentration, floor ( $\mu\text{g}/\text{mg}$ )  
 $SVOCDust_{floor\_avg}$  = Average SVOC in dust concentration, floor ( $\mu\text{g}/\text{mg}$ )  
 $FracTime$  = Fraction of time in environment (unitless)  
 $DustIng$  = Dust ingestion rate (mg/day)  
 $BW$  = Body weight (kg)  
 $CF$  = Conversion factor (1000  $\mu\text{g}/\text{mg}$ )

$$ADR = \frac{(SVOCRP_{floor\_max} + SVOCDust_{floor\_max}) \times FracTime \times DustIng}{BW \times CF} \quad (70)$$

Where:

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

The above equations assume the SVOCs are volatilized from the SVOC-containing article to the air and then partition to dust. Alternately, SVOCs can partition directly from the article to dust in direct contact with the article. This is also

estimated in A\_ING3 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 E6. The model assumes partitioning behavior dominates, or instantaneous equilibrium is achieved. This is presented as a worst-case or upper bound scenario.

$$C_d = \frac{C_{0\_art} \times K_{dust} \times \rho_{dust}}{K_{solid}} \quad (71)$$

Where:

- $C_d$  = Concentration of SVOC in dust (mg/cm<sup>3</sup>)
- $C_{0\_art}$  = Initial SVOC concentration in article (mg/cm<sup>3</sup>)
- $K_{dust}$  = SVOC dust-air partition coefficient (m<sup>3</sup>/mg)
- $\rho_{dust}$  = Dust density (mg/m<sup>3</sup>)
- $K_{solid}$  = Solid air partition coefficient (unitless)

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

$$CADD_{DTD} = \frac{C_d \times \text{FracTime} \times \text{DustIng} \times CF}{\rho_{dust} \times BW} \quad (72)$$

Where:

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

$$ADR_{DTD} = \frac{C_d \times \text{FracTime} \times \text{DustIng} \times CF}{\rho_{dust} \times BW} \quad (73)$$

Where:

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

## P\_DER1a: Dermal Dose from 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 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/cm<sup>2</sup>-event) is the product of the film thickness of the liquid on the skin's surface and the density of the formulation.

$$AR = FT \times \rho \quad (74)$$

Where:

*AR* = Amount retained on the skin (g/cm<sup>2</sup>)

*FT* = Film Thickness (cm)

$\rho$  = Density of formulation (g/cm<sup>3</sup>)

$$CADD = \frac{AR \times \frac{SA}{BW} \times FQ_{cr} \times FR_{abs} \times Dil \times WF \times ED_{cr} \times CF_1}{AT_{cr} \times CF_2} \quad (75)$$

Where:

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

*AR* = Amount retained on the skin (g/cm<sup>2</sup>-event)

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

*FQ<sub>cr</sub>* = Frequency of use, chronic (events/year)

*FR<sub>abs</sub>* = Absorption fraction (unitless)

*Dil* = Product dilution fraction (unitless)

*WF* = Weight fraction of chemical in product (unitless)

*ED<sub>cr</sub>* = Exposure duration, chronic (years)

*CF<sub>1</sub>* = Conversion factor (1000 mg/g)

*AT<sub>cr</sub>* = Averaging time, chronic (years)

*CF<sub>2</sub>* = Conversion factor (365 days/year)

$$ADR = \frac{AR \times \frac{SA}{BW} \times FQ_{ac} \times FR_{abs} \times Dil \times WF \times ED_{ac} \times CF_1}{AT_{ac}} \quad (76)$$

Where:

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

*AR* = Amount retained on the skin (g/cm<sup>2</sup>-event)

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

- $FQ_{ac}$  = Frequency of use, acute (events/day)  
 $FR_{abs}$  = Absorption fraction (unitless)  
Dil = Product dilution fraction (unitless)  
 $WF$  = Weight fraction of chemical in product (unitless)  
 $ED_{ac}$  = Exposure duration, acute (days)  
 $CF_1$  = Conversion factor (1000 mg/g)  
 $AT_{ac}$  = Averaging time, acute (days)

### Estimating $FR_{abs}$

The fraction absorbed ( $FR_{abs}$ ) can be chosen by one of two methods:

1. Entering a fraction absorbed,
2. Using the “Estimate” button and having the model calculate the fraction absorbed using the following equation ([Frasch and Bunge, 2015](#)):

$$FR_{abs} = \frac{3 + \chi \left[ 1 - \exp\left(-\alpha \frac{t_{exp}}{t_{lag}}\right) \right]}{3(1 + \chi)} \quad (77)$$

- $\chi$  = Ratio of the evaporation rate from the SC surface to the dermal absorption rate through the SC (unitless)  
 $\alpha$  = Constant (2.906)  
 $t_{exp}$  = Exposure time (h)  
 $t_{lag}$  = Lag time for chemical transport through the SC (h)

Where  $t_{lag}$  is defined as:

$$t_{lag} = \frac{h_{SC}}{(6 \times 10^{-2.8 - 0.0056MW})} \quad (78)$$

- $h_{SC}$  = Stratum corneum thickness (assumed to be 15  $\mu\text{m}$ )  
 $MW$  = Molecular weight (mg/mmol)

Where  $\chi$  is defined as:

$$\chi = \frac{h \times P_{vap} \times MW \times CF_1}{K_p \times S_W \times R \times T} \quad (79)$$

- $h$  = Gas phase mass transfer coefficient (m/h)  
 $P_{vap}$  = Vapor Pressure (Torr)

- $MW$  = Molecular weight (mg/mmol)
- $K_p$  = Permeability coefficient for chemical transport through the SC from an aqueous vehicle (cm/h)
- $S_w$  = Water solubility (mg/mL)
- $R$  = Real gas constant (62.37 mL-Torr/K-mmol)
- $T$  = Temperature (Kelvin)
- $CF_1$  = Conversion factor (100 cm/m)

The permeability coefficient ( $K_p$ ) in Equation 79 is estimated using the built in CEM estimator from P\_DER1b (Equation 80). The gas phase mass transfer coefficient ( $h$ ) is estimated using Equation 47.

### P\_DER1b: Dermal Dose from 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:

3. Entering a permeability coefficient
4. Using the “Estimate” button and having the model calculate the permeability coefficient using the following equation ([ten Berge, 2010](#)):

$$K_p = \frac{1}{\left(\frac{1}{K_{lip} + K_{pol}}\right) + \left(\frac{1}{K_{aq}}\right)} \quad (80)$$

Where,

- $K_p$  = Permeability coefficient for chemical transport through the SC from an aqueous vehicle (cm/h)
- $K_{lip}$  = Permeation coefficient of the lipid medium
- $K_{pol}$  = Permeation coefficient of the protein fraction of the SC
- $K_{aq}$  = Permeation coefficient of water (epi)dermal layer

Where  $K_{lip}$ ,  $K_{pol}$  and  $K_{aq}$  are defined in Equations 81-83, respectively,

$$K_{lip} = 10^{(-2.96 + 0.981 \times \log(K_{ow}) - 0.0079 \times MW)} \quad (81)$$

$$K_{pol} = \frac{0.0552}{MW^{1.38}} \quad (82)$$

$$K_{aq} = \frac{1121}{MW^{1.96}} \quad (83)$$

$$CADD = \frac{K_p \times D \times Dil \times \rho \times \frac{SA}{BW} \times FQ_{cr} \times WF \times ED_{cr} \times CF_1}{AT_{cr} \times CF_2} \quad (84)$$

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)
- $\rho$  = Density of formulation (g/cm<sup>3</sup>)
- $\frac{SA}{BW}$  = Surface area to body weight ratio (cm<sup>2</sup>/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)

$$ADR = \frac{K_p \times D \times Dil \times \rho \times \frac{SA}{BW} \times FQ_{ac} \times WF \times ED_{ac} \times CF_1}{AT_{ac}} \quad (85)$$

Where:

- $ADR$  = Potential Acute Dose Rate (mg/kg-day)
- $K_p$  = Permeability coefficient (cm/hr)
- $D$  = Duration of use (hr/event)
- $Dil$  = Product dilution fraction (unitless)
- $\rho$  = Density of formulation (g/cm<sup>3</sup>)
- $\frac{SA}{BW}$  = Surface area to body weight ratio (cm<sup>2</sup>/kg)
- $FQ_{ac}$  = Frequency of use, acute (events/day)
- $ED_{ac}$  = Exposure Duration, acute (days)
- $WF$  = Weight fraction of chemical in product (unitless)
- $CF_1$  = Conversion factor (1000 mg/g)
- $AT_{ac}$  = Averaging time, acute (days)

## P\_DER2: Dermal Dose from Soil where Skin Contact with Soil, Dust, or Powder Occurs

The model for exposure to products mixed with soil and powdered products is similar to the model of dermal exposure of settled dust (A\_DER3). The equation models general exposure to chemicals from powdered solids such as soil, dust or powdered chemicals (Pawar et al. 2016). For scenarios with powdered products, the user must provide the concentration of the chemical in the products.

CEM has a built in estimator to calculate the concentration of the chemical in soil for scenarios with products added to soil. The estimator takes into account chemical decay in the soil. Equations 86 and 87 estimate the concentration of a chemical in soil to be used in CADD and ADR:

$$C_{soil,cr} = \frac{M \times WF \times CF_m \times \left(\frac{1}{253/t_{1/2}}\right) \times \left(1 - e^{-\left(\frac{253}{t_{1/2}}\right)}\right)}{Area \times Depth \times \rho \times (1 - \emptyset)} \quad (86)$$

Where:

- $C_{soil,cr}$  = Concentration of chemical in soil (mg/kg)
- M = Mass of product used per application (g)
- WF = Weight fraction (unitless)
- $t_{1/2}$  = Chemical half-life in soil
- Area = Area of yard product is applied (m<sup>2</sup>)
- Depth = Mixing depth of soil (m)
- $\rho$  = Soil density (kg/m<sup>3</sup>)
- $\emptyset$  = Soil porosity (unitless)
- $CF_m$  = Conversion factor (1000 mg/g)

$$C_{soil,ac} = \frac{M \times WF \times CF_m \times \left(\frac{1}{0.69/t_{1/2}}\right) \times \left(1 - e^{-\left(\frac{0.69}{t_{1/2}}\right)}\right)}{Area \times Depth \times \rho \times (1 - \emptyset)} \quad (87)$$

Where:

- $C_{soil,ac}$  = Concentration of chemical in soil (mg/kg)
- M = Mass of product used per application (g)
- WF = Weight fraction (unitless)
- $t_{1/2}$  = Chemical half-life in soil
- Area = Area of yard product is applied (m<sup>2</sup>)
- Depth = Mixing depth of soil (m)
- $\rho$  = Soil density (kg/m<sup>3</sup>)
- $\emptyset$  = Soil porosity (unitless)

$CF_m$  = Conversion factor (1000 mg/g)

$$CADD = \frac{C_{soil} \times \frac{SA}{BW} \times AF \times FA \times FQ_{cr} \times ED_{cr}}{CF_1 \times CF_2 \times AT_{cr}} \quad (88)$$

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

$C_{soil}$  = Concentration in soil, dust or powder (mg/kg)

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

$AF$  = Adherence factor of dust to hand (mg/cm<sup>2</sup>-event)

$FA$  = Fraction absorbed (unitless)

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

$CF_1$  = Conversion factor (10,000 mg/kg)

$CF_2$  = Conversion factor (365 days/yr)

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

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

$$ADR = \frac{C_{soil} \times \frac{SA}{BW} \times AF \times FA \times FQ_{ac} \times ED_{ac}}{CF_1 \times AT_{ac}} \quad (89)$$

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

$C_{soil}$  = Concentration in soil, dust, or powder (mg/kg)

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

$AF$  = Adherence factor of soil or product to hand (mg/cm<sup>2</sup>-event)

$FA$  = Fraction absorbed (unitless)

$FQ_{ac}$  = Events per day (events/day)

$CF_1$  = Conversion factor (1000 ug/mg)

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

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

### **A\_DER1: Dermal Dose from Direct Transfer from Vapor Phase to Skin (Article Model)**

Chemicals within the vapor phase can partition directly to the skin, resulting in dermal exposure. In this 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):

$$K_{p\_cw} = 10^{(0.7 \times \text{Log}K_{ow} - 0.0722 \times MW^{\frac{2}{3}} - 5.252)} \quad (90)$$

$$K_{p\_w} = \frac{K_{p\_cw}}{1 + (K_{p\_cw} \times MW^{0.5}) / 2.6} \quad (91)$$

$$K_{p\_b} = \frac{K_{p\_w}}{40.9 \times H} \quad (92)$$

$$K_{p\_g} = \left( \frac{1}{V_d} + \frac{1}{K_{p\_b}} \right)^{-1} \quad (93)$$

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)

$$DerFlux = \frac{K_{p\_g} \times C_g}{CF} \quad (94)$$

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 ( $10000 \text{ cm}^2/\text{m}^2$ )

$$\log(K_{L\_g}) = 0.74 + \log(K_{ow}) + \log(H) + \log(RT) \quad (95)$$

Where:

- $K_{L\_g}$  = Gas-phase to skin lipid partitioning coefficient (unitless)

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

$$CADD = \frac{DerFlux \times \frac{SA}{BW} \times FracTime \times ED_{cr} \times CF_1}{AT_{cr} \times CF_2} \quad (96)$$

Where:

- $CADD$  = Potential Chronic Average Daily Dose (mg/kg-day)  
 $DerFlux$  = Dermal flux ( $\mu\text{g}/\text{cm}^2\text{-hr}$ )  
 $\frac{SA}{BW}$  = Surface area to body weight ratio ( $\text{cm}^2/\text{kg}$ )  
 $FracTime$  = 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  $\mu\text{g}/\text{mg}$ )

$$ADR = \frac{DerFlux \times \frac{SA}{BW} \times FracTime \times ED_{ac} \times CF_1}{AT_{ac} \times CF_2} \quad (97)$$

Where:

- $ADR$  = Potential Acute Dose Rate (mg/kg-day)  
 $DerFlux$  = Dermal flux ( $\mu\text{g}/\text{cm}^2\text{-hr}$ )  
 $\frac{SA}{BW}$  = Surface area to body weight ratio ( $\text{cm}^2/\text{kg}$ )  
 $FracTime$  = 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  $\mu\text{g}/\text{mg}$ )

## A\_DER2: Dermal Dose from Skin Contact with Article

This model calculates the dermal exposure due to migration of a chemical within an article to the skin via direct article contact. The model is based on a simplified diffusion model employed by [Delmaar et al. 2013](#) to estimate dermal dose after the diffusion of substances in articles to the surface of the article. This equation is a physically-based emission model, grounded in the well-established theory of diffusion of substances in materials. The chemical is modeled as emitted from the source to the skin directly, driven by diffusion through the material. Based on Delmaar et al. 2013, the average distance,  $l$ , a diffusing molecule will travel during contact,  $Dur$ , is calculated by the equation:

$$l = \left( \sqrt{2 \times (D \times 60) \times Dur} \right) \times CF_1 \quad (98)$$

Where:

- $l$  = Average distance a diffusing molecule travels per contact (cm)
- $D$  = Solid phase diffusion coefficient (m<sup>2</sup>/hr)
- $Dur$  = Duration of article contact (min)
- $CF_1$  = Conversion factor (100 cm/m)

Once the average distance per contact is calculated then the chronic dose rate can be calculated.

$$CADD = \frac{C_{art} \times \frac{SA}{BW} \times l \times N \times ED_{cr}}{AT_{cr}}$$

Where:

- $CADD$  = Potential Chronic Average Daily Dose (mg/kg-day)
- $C_{art}$  = Chemical concentration in article (mg/cm<sup>3</sup>)
- $\frac{SA}{BW}$  = Surface area to body weight ratio (cm<sup>2</sup>/kg)
- $N$  = Number of contacts with article per day (day<sup>-1</sup>)
- $ED_{cr}$  = Exposure duration, chronic (years)
- $AT_{cr}$  = Averaging time, chronic (years)

$$ADR = \frac{C_{art} \times \frac{SA}{BW} \times l \times N \times ED_{ac}}{AT_{ac}} \quad (99)$$

Where:

- $ADR$  = Potential Acute Dose Rate (mg/kg-day)
- $C_{art}$  = Chemical concentration in article (mg/cm<sup>3</sup>)
- $\frac{SA}{BW}$  = Surface area to body weight ratio (cm<sup>2</sup>/kg)
- $N$  = Number of contacts with article per day (day<sup>-1</sup>)
- $ED_{ac}$  = Exposure duration, acute (days)
- $AT_{ac}$  = Averaging time, acute (days)

### A\_DER3: Dermal Dose from Skin Contact with Articles using Dust Concentration

Chemicals from articles can partition to the dust that lies on article surface. This can result to dermal exposure through contact with dust settled on top of articles. The equation uses the concentration of the chemical in settled dust calculated from the SVOC Model (see Equation 42). The CADD equation uses the average floor dust concentration, while for ADR the maximum floor dust concentration is used.

$$CADD = \frac{F_{dust} \times \frac{SA}{BW} \times AF \times FA \times EvD \times ED_{cr}}{CF_1 \times AT_{cr}} \quad (100)$$

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

*F<sub>dust</sub>* = Average floor dust SVOC concentration (ug/mg)

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

AF = Adherence factor of dust to hand (mg/cm<sup>2</sup>-event)

FA = Fraction absorbed (unitless)

EvD = Frequency of article contact per day (events/day)

*CF<sub>1</sub>* = Conversion factor (1000 ug/mg)

*ED<sub>cr</sub>* = Exposure duration, chronic (years)

*AT<sub>cr</sub>* = Averaging time, acute, chronic (years)

$$ADR = \frac{F_{dust} \times \frac{SA}{BW} \times AF \times FA \times EvD \times ED_{ac}}{CF_1 \times AT_{ac}} \quad (101)$$

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

*F<sub>dust</sub>* = Maximum floor dust SVOC concentration (ug/mg)

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

AF = Adherence factor of dust to hand (mg/cm<sup>2</sup>-event)

FA = Fraction absorbed (unitless)

EvD = Frequency of article contact per day (events/day)

*CF<sub>1</sub>* = Conversion factor (1000 ug/mg)

*ED<sub>ac</sub>* = Exposure duration, acute (days)

*AT<sub>ac</sub>* = Averaging time, acute (days)

## 4. Areas for Future Enhancements

CEM has been enhanced to include additional exposure pathways and scenarios. However, there are still several exposure pathways that are not yet included within CEM.

### Exposure Metrics for Short-term Exposure

Throughout the user guide of CEM, EPA provides metrics of Acute Dose Rates that are averaged over one day, Chronic Average Daily Doses that are averaged over one year, and Lifetime Average Daily Doses and Concentrations that are averaged over a lifetime (78 years). Further consideration could be given to additional short-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 µg/m<sup>3</sup>). Applying a uniform value to “stop” an event across chemicals/scenarios such as 0.001 µg/m<sup>3</sup> or 1 ng/m<sup>3</sup> could be considered. Note, averaging periods for user-defined time periods can be calculated manually using the intermediates report. However, this was not automated within CEM.

### Products used in Water (Appliances, Bathing or Showering)

Additional models may be considered to quantify emission from water to air from appliances or during bathing and showering. Models were identified and summarized below. The generic emission model was added to the IECCU model.

Type of Water source	Reference
Generic	Lyman (1990), Guo (2002)
Showering	Chen et al. (2003)
	Uddameri and Venkataraman (2013)
Bathtub <sup>a</sup>	U.S. EPA (2000)
Washing machine <sup>b</sup>	Howard and Corsi (1998)
Kitchen sink	Howard and Corsi (1996)
Dishwasher	Howard et al. (1999)
Humidifier	Highsmith et al. (1992)
Multiple (Total Exposure Model)	Wilkes et al. (2002)

a This bathtub model includes three models: bathtub flow through, bathtub fill and bathtub surface volatilization.

b This washing machine model includes a fill-cycle and a wash/rinse cycle.

For dermal exposure, the EPA SWIM Model (2003) and a model from the EPA Dermal Exposure Assessment (2007) could be combined and harmonized with the existing CEM dermal models to produce Equation 102 and 103. There are two new parameters, the mass of product used per event (*M*) and the amount of water used per event (*Q*). The mass of product used is already included within CEM and the amount of water is also generally available.

$$CADD = \frac{K_p \times M \times D \times \frac{SA}{BW} \times FQ_{cr} \times ED_{cr} \times CF_1}{Q \times AT \times CF_2 \times CF_3} \quad (102)$$

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

$K_p$  = Dermal permeability coefficient (cm/hr)

M = Amount of product used (mg/event)

D = Event duration (min/event)

SA = Skin surface area available for contact (cm<sup>2</sup>)

BW = Body weight (kg)

$ED_{cr}$  = Exposure duration (yr)

$CF_1$  = Conversion factor (hr/60 min)

Q = Amount of water used per event (gallons/event) for bathing and rate of water use for showering  
and handwashing (gallons/min) x event duration (min/event)

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

$CF_2$  = Conversion factor (0.000264172 cm<sup>3</sup>/gallons)

$CF_3$  = Conversion factor (365 days/yr)

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

$$FQ_{cr} = EV \times EF \quad (103)$$

EV = Event frequency (events/day)

EF = Exposure frequency (days/year)

### Articles in Routine Contact with Water

Water generally 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. Other models such as I-SVOC or use of empirically-based approaches can be considered for these exposure pathways.

### 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.

$$C = \left[ \frac{M \times WF \times F \times N \times CF}{Q} \right] \times R \times SDF \quad (104)$$

- $C$  = 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 (L/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 that 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 the science 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, assuming 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  $\mu\text{g}/\text{cm}^2/\text{hour}$ . EPA has compiled these into a spreadsheet along with chemical concentration in the article to provide a range of possible values to select for this parameter. 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 ( $\sim 37^\circ\text{C}$  for human mouth), pH ( $\sim 6.5$  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.

### **Consideration of Additional Exposure Scenarios and Exposure Defaults**

EPA may consider additional information to modify an existing exposure scenario or add new exposure scenarios as use patterns change. Exposure scenarios are defined for consumer products and articles vary in exposure models from

around the world. Use of consumer products 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.*

**Absorption Fraction;  $FR_{abs}$  (unitless)** Fraction of chemical that is applied to the skin that is absorbed into the skin. Used to estimate dermal exposure to products.

**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](#))

**Airborne Concentration ( $\mu\text{g}/\text{m}^3$ )** Estimated or user-supplied concentration of the chemical in the room (**Zone 1**) or in the portion of the building that is not the room (**Zone 2**) in which the product or article is used.

**Air Exchange Rate (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 (**Zone 1**) or for the portion of the building where the product or article is not in use (**Zone 2**) [([U.S. EPA, 2011](#)) Table 19-24].

**Air exchange rate between the near field and far field ( $\text{m}^3/\text{min}$ )** 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.

**Ambient Particulate Concentration ( $\text{mg}/\text{m}^3$ )** 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;  $AR$  ( $\text{g}/\text{cm}^2$ )** 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 ( $\text{g}/\text{cm}^3$ ).

**Application time;  $t_a$  (min)** The time of product use. This value is calculated from the duration of product use and is used in the model to estimate airborne emission rates.

**Area of Interior Surfaces;  $A_{Int}$  ( $\text{m}^2$ )** The surface area of interior surfaces such as furnishings and building materials that are potential sinks for airborne SVOCs.

**Area of Yard ( $\text{m}^2$ )** 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).

**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.

**Change in Concentration with Time;  $\frac{\partial C}{\partial t}$  ( $\mu\text{g}/\text{m}^3/\text{hr}$ )** The change in the chemical concentration in air over time within a zone.

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

**Cleaning Efficiency (unitless)** The time period for one-half of the original product mass applied to the ground to decay due to environmental fate processes. 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 Periodicity ( $\text{hr}^{-1}$ )** 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 as default values 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).

**Concentration ( $\text{mg}/\text{m}^3$ )** Measure of chemical in units of mass per volume either in the product or article or exposure media (air, particles, dust, soil.)

**Contact Area of Mouthing; CA, ( $\text{cm}^2$ )** The area of an article that comes into contact with mouth.

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

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

**Density of Formulation or Product;  $\rho$  ( $\text{g}/\text{cm}^3$ )** The density of the product formulation or article material. This is used by CEM for other calculations.

**Density of RP;  $\rho_{RP}$  ( $\text{mg}/\text{m}^3$ )** Density of respirable particles based on value recommended in (Little et al., 2012).

**Density of Soil ( $\text{mg}/\text{m}^3$ )** Density of soil used by CEM in calculating exposure from products applied to ground.

**Deposition Rate, Dust;  $kdep_{Dust}$  ( $\text{hr}^{-1}$ )** 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  $10\ \mu\text{m}$  (10–25 and >25) were averaged and rounded to the nearest tenth [(U.S. EPA, 2011); Table 19-33].

**Deposition Rate, RP;  $k_{dep_{TSP}}$  ( $hr^{-1}$ )** 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 RP, the deposition rates for particles less than 10  $\mu m$  (1-5 and 5-10) were averaged and rounded to the nearest tenth [([U.S. EPA, 2011](#)); Table 19-33].

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

**Diffusion Coefficient ( $m^2/hr$ )** 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 Mouthing;  $D$  ( $hr/event$ )** The amount of time that an article is mouthed.

**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 Fraction;  $IF_{Dust}$  (unitless)** An estimate inhaled airborne particles in the dust size range that are ingested. Values must be between 0 and 1. The default value is 1 and should be used unless data are available.

**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.

**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](#)).

**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.

**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" (E2), 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 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 dust (large particles.)

**Fraction Organic Matter RP (unitless)** Fraction of organic matter in respirable (small) particles.

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

**Frequency of Use/Application, 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/Application, 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.

**Frequency of Mouthing;  $FQ$  (events/day)** The number of times an object is mouthed (or mouth to object contact is made) daily.

**Henry's Law Coefficient (atm/M)** 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  $\mu\text{m}$ ) ([Creech et al., 1996](#)).

**HVAC Penetration Efficiency for RP (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 Rate of Dust (mg/day)** Daily dust ingestion rate. Dust is defined as particles that exist within the home, and may be comprised of soil. Default values by age group are from EPA's Exposure Factors Handbook ([U.S. EPA, 2011](#)).

**Ingestion Rate of Soil (mg/day)** Daily incidental soil ingestion rate. Soil is comprised of particles that exist outdoors. Default values by age group are from EPA's Exposure Factors Handbook ([U.S. EPA, 2011](#)).

**Inhalation Rate ( $\text{m}^3/\text{hr}$ )** 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 ( $\text{m}^3/\text{hr}$ )** 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 ( $\text{m}^3/\text{hr}$ )** 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 ( $\text{mg}/\text{m}^3$ )** The SVOC additive concentration in a consumer article.

**Interzonal Air Flow Rate ( $\text{m}^3/\text{hr}$ )** The volumetric air flow between Zones 1 and 2 during and after product usage.

**Lifetime Average Daily Concentration; LADC (mg/kg-day)** Estimated average daily airborne concentration of a chemical averaged over both use and non-use days.

**Lifetime Average Daily Dose; LADD (mg/kg-day)** The average daily dose calculated over a lifetime.

**Loading (g/cm<sup>2</sup>)** The amount of chemical on the surface of a mouthed article or skin. CEM provides default values for many products and articles. These can be modified by the user.

**Mass Generation Rate, 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 mg/m<sup>2</sup>/day and 2.5, respectively. The mat used in the study for dirt collection was 0.318 m<sup>2</sup>, 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](#)).

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

**Mass Generation Rate, 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 hr; children under 5: 21.5 hr
- 90th percentile: adults: 23 hr; children under 5: 24 hr

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 m<sup>2</sup>
- Children: 0.6 m<sup>2</sup>

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

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

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

- *Low* = 2 × adult median
- *Medium* = 2 × adult median + 2 × child median
- *High* = 2 × Adult 90th + 2 × child 90th

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

**Mass Generation Rate, Suspended RP (mg/hr)** Generation rate for fine particulates inside the home. The PM<sub>10</sub> 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.

NOTE: Mass Generation Rate of dust and RP into air and onto floor is in mg/hr ( $g_{ATSP}$ ;  $g_{ADust}$ ;  $g_{FTSP}$ ;  $g_{FDust}$ ).

**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.

**Migration Rate of Chemical from Article to Saliva;  $MR$  (mg/cm<sup>2</sup>/hr)** A measure of the flux in mass per area per time of a chemical from an article containing the chemical to the saliva during mouthing. This is a function of the chemical and the article itself and, along with mouthing behaviors such as frequency, area, and duration, governs mouthing exposure.

**Mixing Depth of Soil;  $Depth$ , (m)** Maximum depth in which a chemical can be expected to be mixed in soil after application of the chemical to the surface of the soil. For example, tilled soiled will have a greater mixing depth and a lower resulting soil concentration than soiled that are not mechanically mixed.

**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.

**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;  $K_p$  (m/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;  $\phi$  (unitless)** A measure of the porosity, or air spaces, in soil.

**Potential Peak Concentration (mg/m<sup>3</sup>)** 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 ratio of the product that is diluted for use, for example, cleaning products that are diluted in water. Values must be between 0 and 1.

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

**Radius of RP;  $r_{RP}$  (m)** Radius of respirable particles ([Little et al., 2012](#)).

**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  $\mu\text{m}$  (10-25 and >25) were averaged and rounded to two significant digits [([U.S. EPA, 2011](#)); Table 19-33].

**Resuspension Rate, RP (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 RP, the resuspension rates for particles less than 10  $\mu\text{m}$  (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].

**RP Ingestion Fraction;  $IF_{RP}$  (unitless)** An estimate inhaled airborne particles in the respirable particle size range that are ingested. Values must be between 0 and 1. The default value is 0 and should be used unless data are available.

**Saturation Concentration in Air ( $\mu\text{g}/\text{m}^3$ )** 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 is employed within the dermal air-to-skin model (A\_DER1).

**Surface Area of Article (m<sup>2</sup>)** 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, caution 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 ( $m^2$ )** 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 ( $m^2$ )** 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.

**Surface Area to Body Weight Ratio;  $\frac{SA}{BW}$  ( $cm^2/kg$ )** For products, the ratio of the surface area of the body in contact with the product to body weight. For articles, 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.

**SVOC Gas-Phase Concentration in Contact with Article Surface ( $\mu g/m^3$ )** 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. CEM uses the saturation vapor pressure in the absence of any monitoring data.

**SVOC in RP Concentration;  $SVOC_{RP}$  ( $\mu g/mg$ )** The ratio of the mass of SVOC sorbed to respirable particles to the mass of the respirable particle. Used to estimate inhalation and ingestion exposure of particle-bound SVOCs.

**SVOC in Dust Concentration;  $SVOC_{Dust}$  ( $\mu g/mg$ )** The ratio of the mass of SVOC sorbed to large particles to the mass of the respirable particle. Used to estimate inhalation and ingestion exposure of particle-bound SVOCs.

**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;  $K_{Dust}$  ( $m^3/mg$ )** 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 RP-Air Partition Coefficient;  $K_{RP}$  ( $m^3/mg$ )** 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.

**Thickness of the Solid Layer;  $L$  (m)** The thickness of the solid layer may be assumed to be 0.005 m for interior surfaces and equal to the radius of the particle for particulates. Solid refers to where 'solid' refers to indoor sink (int), respirable particles (RP), or dust.

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

**Temperature (K)** The temperature of the indoor environment.

**Transfer Coefficient ( $\text{cm}^2/\text{hr}$ )** A measure of the rate of transfer of a chemical on a surface to the skin.

**Transfer Coefficient ( $\text{cm}^2/\text{hr}$ )** An estimate of the transfer of chemical on the surface of the article to skin. The default values from the OPPT residential scenarios 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).

**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.

**Ventilation Rate;  $Q$  ( $\text{m}^3/\text{hr}$ )** Volumetric rate of air exchange between building zones or between a building zone and the outdoors. Used in conjunction with the zone volume to calculate air exchange rates.

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

**Volume of Building ( $\text{m}^3$ )** The total volume of all rooms in the home or other building where the product or article is used. Building volume is used 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].

**Volume of Room ( $\text{m}^3$ )** The total volume of the room of product use in the home or other building where the product or article is used. Room volume is used to estimate air concentrations of the chemical in Zone 1 (i.e., room where the product or article is in use) [([U.S. EPA, 2011](#)), Table 19-6].

**Volume of Far Field ( $\text{m}^3$ )** 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.

**Volume of Near Field ( $\text{m}^3$ )** 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](#)).

**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.

## References

**The reference list includes references from the CEM User Guide document and CEM Appendices.**

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