Consumer Exposure Model

Consumer Exposure Model (CEM)

User Guide

Prepared for EPA Office of Pollution Prevention and Toxics

by ICF

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Executive Summary

OPPT aims for CEM to be 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 defaults currently included in CEM are based on available data and professional judgment and are present in order for model users to have the ability to use all parts of the model without requiring the model user to determine all model inputs for each model run. At any time, defaults, chemicals, or use scenarios could 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 fifteen additional models. The updated version now includes six emission models, three inhalation models, five ingestion models, and seven 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 a 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. These values can be estimated from EpiSuite^{TM}. 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 ConsExpo 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.

Following incorporation of peer review comments, Version 2.1 of CEM is completed. Based on the feedback of the peer reviewers, the following changes have been implemented in CEM:

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, 11 generic product categories and one generic article categories were added.
2. New dermal models were added: A_DER2 Dermal Dose from Article where Skin Contact Occurs, P_DER3 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_DER2b was revised and a fraction absorbed estimator was incorporated into P_DER2b. 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. The ability to report Lifetime, in addition to Chronic, Average Daily Dose, was added.
5. Maximum limits were added to restrict users from entering values beyond a reasonable value for certain inputs.
6. Model names were updated to more clearly indicate the model's function.
7. Models within CEM were ground-truthed against existing monitoring data, where available.
8. A sensitivity analysis was completed.
9. The reports in CEM have been refined and reorganized.
10. Users can now access the User's Guide from within CEM.

Additional changes were made to CEM and the User Guide based on EPA feedback:
1. The option to model emission using an emission factor was added.
2. The dermal article contact (A_DER3) model was updated based on stability tests.
3. A vapor to skin for products (P_DER1) model was added.
4. The fraction of chemical removed was added to the fraction absorbed product dermal model (P_DER2a).
5. The average molecule diffusion per contact estimator was corrected.
6. Stability tests for all product/scenario combination were conducted.
7. Prepopulated scenarios were added.
8. Additional product/scenario combinations that were not in previous versions were added.
9. Terminology and terms used within the model and User's Guide were clarified and added to the glossary.
10. Some defaults for certain products and articles were updated.
11. Some surface area to body weight ratios were changed for certain product scenarios.
12. The reports from CEM were updated.

Introduction

Under the Frank R. Lautenberg Chemical Safety in the 21st 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 together with modeling tools to provide scientifically based estimates of exposures and doses.

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

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

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

CEM contains 53 product categories and 20 article categories along with 11 generic product categories and one generic article categories. 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 that a given chemical is present.

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

 Formulations (e.g., weight fraction),
 Use patterns (e.g., frequency, duration, and amount used),
 Human exposure factors (e.g., body weight, inhalation rate),
 Environmental conditions (e.g., air exchange rates and room size), and
 Chemical or product-specific properties (e.g., product density, vapor pressure, molecular weight, diffusion coefficient, overspray fraction, transfer 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 (see Appendix B for more details). The product use, users, and use environment can be modified but not all inputs have complete user flexibility, such as the user and bystander activity patterns.

Based on the data available, OPPT will consider variability and uncertainty associated with model inputs and overlap model outputs. Variation has been incorporated (high, medium, 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. How much of a product is used (amount), how often (frequency), and for how long (duration) vary. This information, when combined with human and built environment exposure factors, can be used for 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 population-based, 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 volatile organic compound (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).[1] You must "unzip" the CEM files before the first use. CEM will not run if you attempt to open and use it from within the zip file (i.e., without unzipping the CEM files). The CEM files may be unzipped to a computer hard drive, network folder, or other storage location. For best performance, it is recommended to unzip CEM to your computer hard drive. Follow the steps below to download, unzip, and open CEM.

1. Download zip file titled "CEM Version 2.1.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.
2. Right click on file and select "Extract All" or "Extract to here" or similar command. The specific command to unzip/extract the file may differ depending on which file compression utility you use (e.g., WinZip, 7-zip).
3. Click "Extract". A new folder will appear where you downloaded the original zip file.
4. Double click the folder to open it and double click the main CEM file titled "CEM Version 2.1.accdb". This folder also includes a copy of this User Guide and two executable files (CEM_NFFF_v29.exe and SVOC14_v3.exe).
5. The first time you open the main CEM file, Windows security will disable the model code. You must click "Enable Content" near the menu bar at the top of the screen to enable the model programming to run. At the top right of the screen, to the right of the CEM logo, select 'View a Saved Analysis' or 'New Analysis' to begin.

Overview

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

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

Instructions for navigating the heading bar and each of the tabs are presented 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.

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

Hiding Access Task Bar
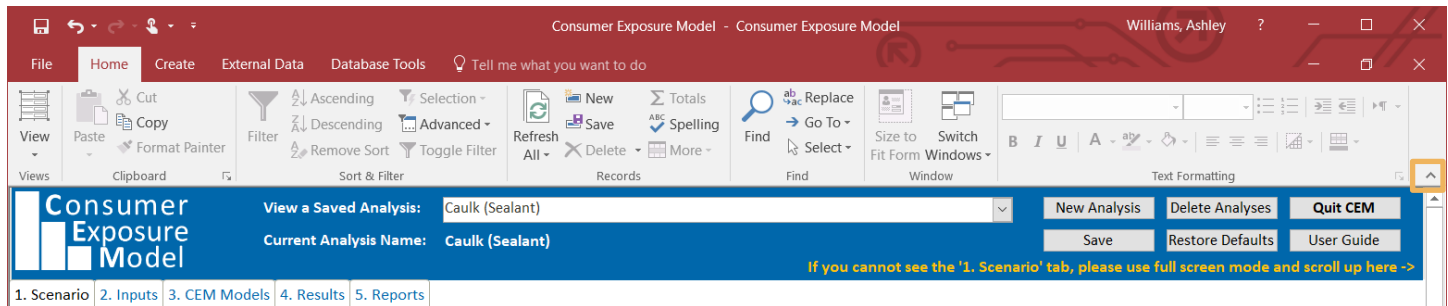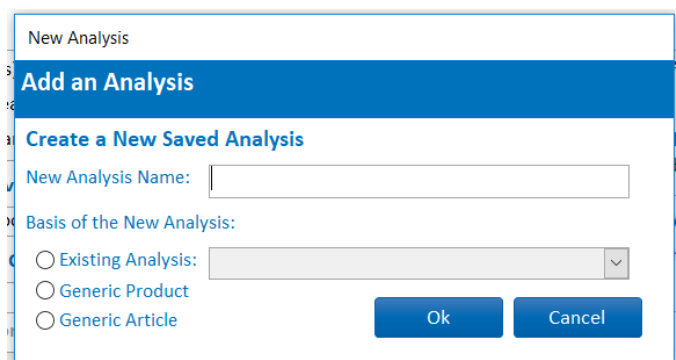
When CEM is opened, the Access Taskbar (that includes, File, Home, Create, External Data, and Database Tools and subheading options underneath each) is automatically visible. These controls are not used by CEM. To hide these and maximize CEM viewing, click the "up" caret on the bottom right side of the 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. View a saved analysis. CEM is pre-loaded with 53 product-specific scenarios, 11 generic product scenarios, 20 article-specific scenarios, and one generic article scenario. Each scenario has defaults already saved within the scenario. Once users create and save their own analyses, they are accessible via the "view a saved analysis" dropdown.

2. Create a new analysis. A new analysis can be created based on a generic product or article or an existing analysis. Currently CEM is populated with one scenario for every product and article category. These scenarios are in turn fully populated with default inputs for that scenario. The modeler can select a chemical to be modeled and change any of the pre-populated inputs. The product and article selections cannot be altered and then saved for pre-populated scenarios. Users can make changes to other defaults associated with pre-populated scenarios and save over them. Users can restore defaults to the original defaults included for a pre-populated scenario by using the "Restore Defaults" button.

Additional controls on the heading bar include:

3. Use the 'Delete Analyses' button to delete one or more previously saved analyses.
4. 'Quit CEM' prompts the user to save any changes to a scenario, and then closes CEM.
5. 'Save' allows users to save changes they make to the current analysis.
6. 'Restore Defaults' restores all fields to the preprogrammed defaults for the current analysis.
7. The 'User Guide' button opens the CEM User Guide.

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

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 53 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 11 generic product and one generic article categories 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 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. **Product/Article 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 environment of use.

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 or Dust 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, A_DER3). The chronic exposure to these media are calculated and reported separately from pathway-specific exposures. These are set to zero as default.

9. **Available 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). 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 details are entered. The Inputs tab includes five subtabs ("a" – "e"), each of which is described below.

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

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

2.a. Chemical Properties Input tab

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

- Vapor pressure,
- Molecular weight,

- Saturation concentration in air,
- Octanol-water partition coefficient,
- Octanol-air partition coefficient,
- Water solubility,
- Henry's Law coefficient, and
- Emission factor.

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 Quantitative Structure-Activity Relationship (QSAR) development, EPA recommends the use of EPI-Suite™ Version 4.11 (U.S. EPA, 2012a) to estimate physical-chemical properties if empirical data are not available. EPI-Suite™ requires either the simplified molecular-input line-entry system (SMILES) code or CAS number/chemical name 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

Chemical Property/Attribute			Estimate All
Chemical Name:		Benzyl Alcohol	
CAS No.:		100516	
Vapor Pressure (torr):	Required	0.094	
Molecular Weight (g/mol):		108.1	
Saturation Concentration in Air (mg/m3):		5.45e+02	1 Estimate
Log Octanol-water Partition Coefficient (-):		1.10E+00	
Log Octanol-air Partition Coefficient (-):		5.96E+00	
Water Solubility (mg/mL):	Not Required	3.30E+01	
Henry's Law Coefficient (atm/M):		3.37E-07	
Emission Factor (ug/m2/hr):		1.60E+06	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,
- 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,
- Skin permeability coefficient,
- Chemical migration rate,
- Surface loading,
- Mouthing transfer efficiency,
- Fraction of chemical that is dislodgeable,
- Product dilution fraction,
- 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

Use the Environment Inputs 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,
- Interzonal ventilation rate,
- Area of interior surface, and
- Thickness of interior surface.

This tab also contains dust parameter inputs (RP, dust, and abraded particle). Examples include:
- Deposition rate (RP, dust, abraded particles),
- Resuspension rate (RP, dust, abraded particles),
- Mass generation rate, suspended (RP, dust, abraded particles),
- Mass generation rate, floor (RP, dust, abraded particles),
- Radius of particle (RP, dust, abraded particles),
- Density of particle (RP, dust, abraded particles),
- Ambient RP concentration,
- Cleaning frequency,
- Cleaning efficiency, and
- HVAC filter penetration.

Other inputs on this tab include near field environment inputs and soil properties which include:
- Near-field volume,
- Far-field volume,
- Air exchange rate at near-field boundary,
- Soil mixing depth,
- Soil density,
- Soil porosity, and
- 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

| 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 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.
4. 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 5th percentile, 50th percentile, and the 95th percentile 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]

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

Receptor-specific Exposure Factors Values for this Analysis [2]

Receptor	Default Value [3]	Analysis Value [4]
Adult (≥21 years)	80	80
Youth (16-20 years)	71.6	71.6
Youth (11-15 years)	56.8	56.8
Child (6-10 years)	31.8	31.8
Small Child (3-5 years)	18.6	18.6
Infant (1-2 years)	12.6	12.6
Infant (<1 year)	7.8	7.8

Restore Defaults

2.e. Activity Patterns Input tab

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

The activity patterns were developed based on human activity diaries included in CHAD. The diaries were used to develop average time spent sleeping and awake, as well as time spent in commercial buildings, government buildings, schools, child occupied facilities (COFs), automobiles, outdoors, and rooms within residences. The diaries were grouped into three bins based on the time spent in residences versus commercial, government, schools, and COFs; average times spent from these three grouping were used to develop the three default activity patterns.

For receptors who are also product users, the default 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

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

1. The Model Selection subtab summarizes the models applicable to the selected product or article. These models are selected by CEM and cannot be edited.

    a. The Model Selection sub-tab includes an option to save intermediate estimates when running inhalation models E1-E6. Intermediates estimates include product use

    schedules, emission rates, contaminant concentrations in air, receptor locations, 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.

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

2. 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.

    a. Clicking on an input will populate information in the Parameter Information pane, on the right side of the page. This text provides an explanation of the clicked variable, sources of automated inputs, and relevant assumptions applied to the input.

Model Selection	E1	P_INH1	P_DER2b	

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)	150
WF	=Weight fraction of chemical in product (-)	0.5
CF	=Conversion factor (mg/g)	1000
ta	= Duration of Use (min/use)	a 120
k	= First-order rate constant for emissions decline (1/min	0.002421
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)   0.002421

Evaporation time, (Eq 3-42)

EvapTime [hr] = 145 / (MW x VP)^0.9546   15.85368

MW	= Molecular Weight (g/mol)	108.1
VP	= Vapor Pressure (torr)	0.094

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:** Caulk (Sealant)	**Chemical Name:** Benzyl Alcohol	☑ 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 LADD/LADC	0.00E+00	2.09E-02	0.00E+00	0.00E+00	0.00E+00	8.19E-02	0.00E+00	1.03E-01
Adult (≥21 years)	8.49E+00	2.85E-02	0.00E+00	0.00E+00	2.73E+01	1.12E-01	3.57E+01	1.41E-01
Youth (16-20 years)	1.00E+01	3.37E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+01	3.37E-02
Youth (11-15 years)	1.17E+01	3.93E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.17E+01	3.93E-02
Child (6-10 years)	1.66E+01	5.58E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.66E+01	5.58E-02
Small Child (3-5 years)	2.38E+01	8.01E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.38E+01	8.01E-02
Infant (1-2 years)	2.93E+01	9.85E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.93E+01	9.85E-02
Infant (<1 year)	3.11E+01	1.05E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.11E+01	1.05E-01

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

5. Reports tab

The Reports tab allows for the viewing and exportation of various reports as PDFs. Four report options are available, including the CEM Results, CEM Results and Inputs, an Inhalation Time-Series Graph, and Inhalation Intermediates. 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.

Inhalation Intermediates report, which may be viewed in Access or exported to Excel, provides the values of selected inputs and calculated results by time step throughout the modeling period. For acute assessments, time-step intermediates are provided for each 30-second time step for 24 hours. The chronic assessment adds hourly intermediate values after the first 24 hours until the end of the 60-day modeling period.

Input values included in the intermediates tables identify when products are or are not in use, and the locations (e.g., bedroom), of adult, youth, and child receptors. Intermediate results include the emission rate, air concentrations in Zones 1 and 2, including near-field and far-field estimates, when applicable. In addition, cumulative intake and exposure estimates are provided for each receptor and zone.

2. Summary of Models within CEM
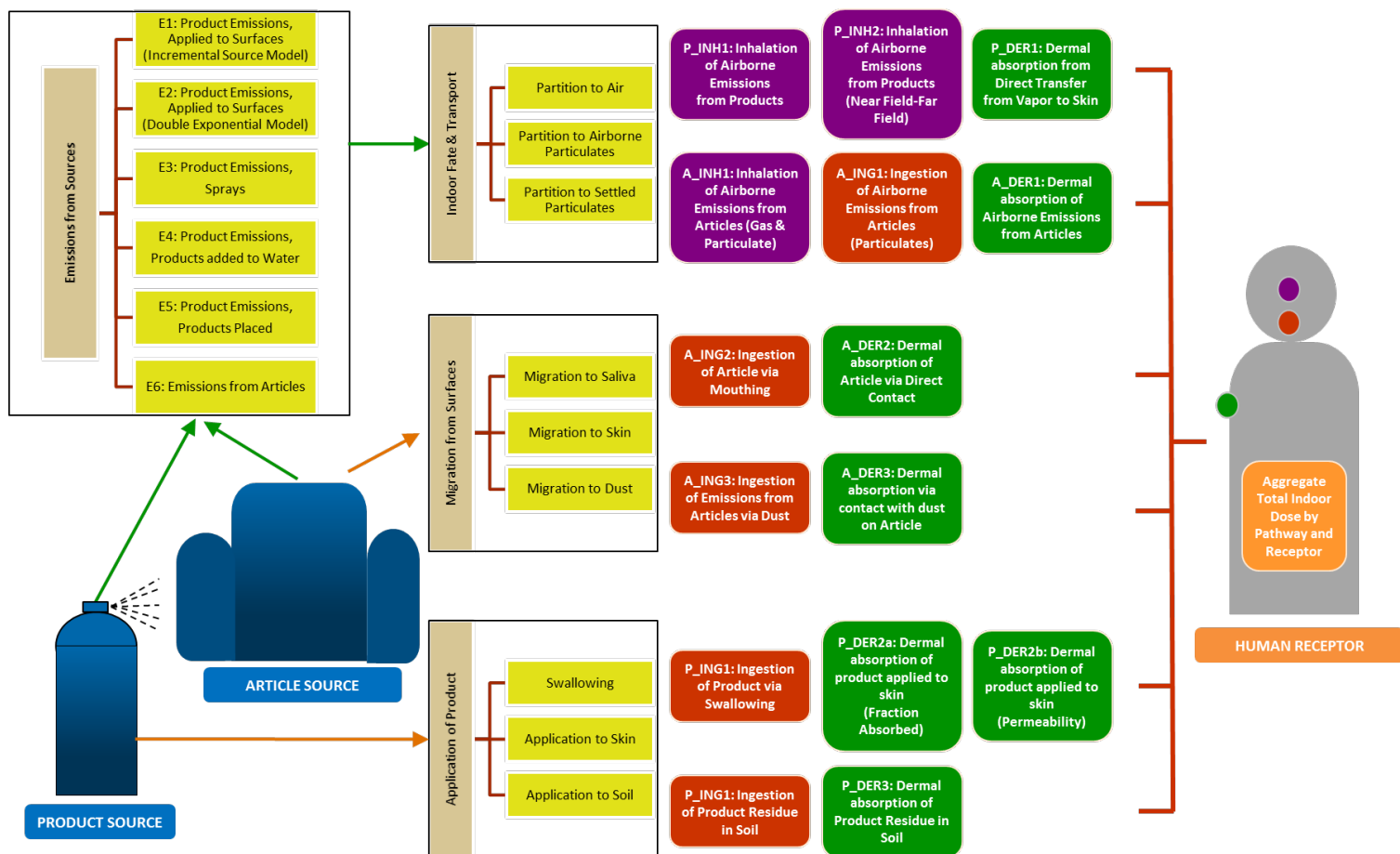
Figure 1. Schematic relationship showing exposure models included in CEM

Figure 1 shows the 21 models within CEM. There are six emission models, three inhalation models (purple), five ingestion models (red), and seven 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 a surface and dry or cure over time, such as paints. Only 25% of the applied mass is released because a substantial fraction of the mass becomes trapped in the cured substrate when it dries. (Note: 10% of the emissions are associated with the first of the double exponential.) Empirical studies

support the assumption of 25% mass released and estimate a relationship between the fast rate of decline and vapor pressure, and between the slow rate of decline and molecular weight. There is a near-field model option that can be selected that seeks to capture the higher concentration in the breathing zone of a product user during use. Alternately, if the near-field option is not selected, Zone 1 is modeled as a homogeneous, well-mixed room. (U.S. EPA, 2007)

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

This 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% 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. The 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

This model assumes emissions of 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 fugacity based model (Little et al., 2012) 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_INH1 is further divided into the near-field, with a default volume of $1m^3$, 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 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 the migration rate is known, the 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 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_DER1: Dermal Dose from Direct Transfer from Vapor Phase to Skin

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 P_INH1 and the partitioning between air and skin lipids, which in turn is dependent on the octanol-air partitioning coefficient, Henry's Law coefficient (or air-water partitioning coefficient), the ideal gas law constant, and temperature (Weschler and Nazaroff, 2012).

P_DER2a: 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, that 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_DER2b: 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_DER3: 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)

Similar to P_DER1, this model describes dermal exposure from gas-phase chemical deposition directly onto the skin from the air, with subsequent absorption. A_INH1 model assumes emissions of SVOC additives from articles and subsequent partitioning between indoor air, airborne particles, and settled dust over time. 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 in turn is dependent on the octanol-air partitioning coefficient, Henry's Law coefficient (or air-water partitioning coefficient), the ideal gas law constant, and temperature (Weschler and Nazaroff, 2012).

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_DER3, 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 E6 are determined in an alternate manner and are described in section E6.)

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 E6, 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:
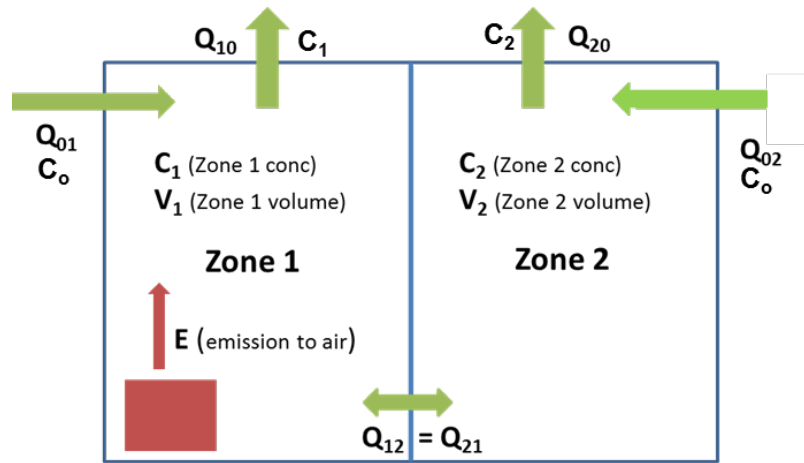
Figure 2. Schematic of two-zone model of indoor environment

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

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

Where:

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

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

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

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

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

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

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

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:

Closed rooms: $\qquad Q_{12} = (0.078 + 0.31 \times AER) \times$ $\hfill$ (3)

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

Where:

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

V $\qquad$ = $\quad$ Volume of building (m^3)

Default volumes for buildings and individual room sizes are taken from the Exposure Factors Handbook (U.S. EPA, 2011). 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. Product-specific scenarios that have a default use environment of outside are: fertilizers, touch up auto paint, de-icing solids, and liquid-based concrete, cement, plaster. There are no product-specific scenarios that have a default use environment of automobile.

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 3 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.
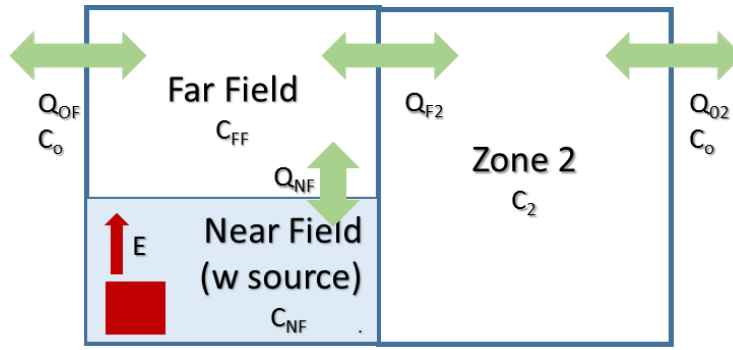
Figure 3. Air flows in the near-field far-field model

Table 1. Guide to Symbols Used in NFFF Model Equations

Symbol	Definition
V_{NF}	Volume of the near-field in Zone 1 (m³)
V_{FF}	Volume of the far-field in Zone 1 (m³)
V_{R2}	Volume of Zone 2 (m³)
Q_{OF}	Ventilation rate of Zone 1 to external environment (m³/hr)
Q_{O2}	Ventilation rate of Zone 2 to external environment (m³/hr)
Q_{f2}	Ventilation rate between Zone 1 and Zone 2 (m³/hr)
Q_{NF}	Ventilation rate between the near field and far field (m³/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

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

Far Field, Zone 1

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

Zone 2

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

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.

The model only exposes the user to the near-field concentration when the product is in use. When the product is no longer in use, the user is exposed to concentration in far-field zone until they change locations based on their activity pattern. For example, if a product is used from 9:00am to 9:20am, the user is in the near-field during use and in the far-field from the end of use until changing locations at 10:00am.

A two-zone model is used only for products that are used in a specific room within the house. For these products, a person is in Zone 1 only when they are in the room of use, either during or after use. A person is in Zone 2 whenever they are in any room other than the room of use. The "whole house" use environment is modeled as a single zone, and a person is in Zone 1 if they are anywhere in the house. If they are not in the house they are neither in Zone 1 nor Zone 2.

For products used outdoors or any other non-residence location, a person is in Zone 1 when in the use environment, and they are never in Zone 2. The outdoor use environment is unique in that it is not an enclosed space. Because CEM is not designed to model air dispersion outdoors, non-users are assumed to be bystanders who receive the same exposure as users.

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). This model is dependent solely on the mass of chemical, rather than the amount of product used. Therefore, dilution is not calculated in this model as it is in dermal models. 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:

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

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 (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):

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

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

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

Users may also estimate k using another method shown in Equations 11 and 12, based on a model to estimate spills using a chemical's gas-phase mass transfer coefficient and parameters of the spill (Guo et al., 2008):

$$k = \frac{E_0}{M_0} \tag{11}$$

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

Where,

E_0	=	Emission factor (µg/m²/hr)
k_g	=	Gas-phase mass transfer coefficient (m/hr)
C_{sat}	=	Saturation concentration based on the vapor pressure of chemical (mg/m³)
M_0	=	Mass of chemical per unit area (µg/m²)

Where,

$$M_0 = \rho \times thickness \times CF_1 \times CF_2$$

$$\tag{13}$$

ρ	=	Density of the chemical (g/cm³)
$thickness$	=	Thickness of the spill/puddle (assumed to be 0.01 cm)
CF_1	=	Conversion factor, 10^4 cm²/m²
CF_2	=	Conversion factor, 10^6 µg/g

Equations 11-13 are used when a user wants to model the emission from a chemical or product spill using an emission factor. If the user selected "Use Emission Factor Method" on the Scenario page, then when a user selects "Estimate All" on the Chemical Properties page, a dialogue box will appear that askes 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

Microsoft Access ✕

Do you want to use the Emission Factor to calculate the decay rate constant for E1?

[Yes] [No]
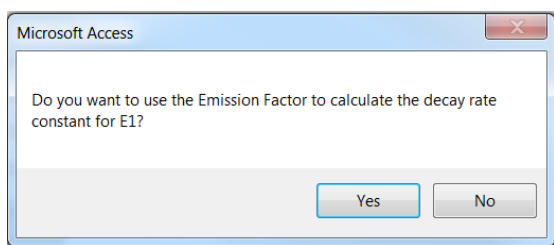
$ER(0)$ can be determined from the fact that the integral of the above $ER(t)$ equation, which accounts for all chemical mass released (i.e., $applied\ mass \times chemical\ weight\ fraction$), is equal to $ER(0) \div k$. However, the equation for the time-varying emission rate resulting from the combination of constant application and exponentially declining emissions (Evans, 1996) requires knowledge of only the total mass released and k.

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

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

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 Pa/mol-K) and T = temperature in Kelvin (298), if an experimentally derived value is not available:

$$C_{sat} = \frac{(VP \times MW \times CF_1 \times CF_2)}{(R \times T)} \tag{15}$$

Where:

C_{sat}	=	Saturation concentration in air (mg/m³)
VP	=	Vapor pressure (Torr)
MW	=	Molecular weight (g/mol)

CF_1 =   Conversion factor, 133 Pa/Torr

CF_2 =   Conversion factor, 10^3 mg/g

R =   Universal gas constant, 8.314 m^3-Pa/mol-K

T =   Temperature (K)

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

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, 1996](#)). This model is dependent solely on the mass of chemical, rather than the amount of product used. Therefore, dilution is not calculated in this model. 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).

$$ER1_1(t) = \frac{M \times WF \times CF}{t_a} \times \left\{ \left[f \times (1 - e^{-k_1(t-t_{start})}) + (1-f) \times \left(1 - e^{-k_2(t-t_{start})} \right) \right] - \left[f \times \left(1 - e^{-k_1(t-(t_{start}+t_a))} \right) + (1-f) \times \left(1 - e^{-k_2(t-(t_{start}+t_a))} \right) \right] \times H(t) \right\} \tag{16}$$

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 $\quad=\quad$ $233.25 \times (VP \div 24) \div 60$ (min^{-1})

k_2 $\quad=\quad$ $0.0000584 \times (MW \div 24) \div 60$ (min^{-1})

VP $\quad=\quad$ Vapor pressure (Torr)

MW $\quad=\quad$ Molecular weight (g/mol)

$$ER_2(t) = \frac{M \times WF \times CF \times (1-f)}{t_a} \times \left[\left(1 - e^{-k(t-t_{start})}\right) - \left(\left(1 - e^{-k(t-(t_{start}+t_a))}\right) \times H(t)\right) \right] \qquad (17)$$

Where:

$ER_2(t)$ $\quad=\quad$ Emission rate at time t (mg/min)

M $\quad=\quad$ Mass of product used (g)

WF $\quad=\quad$ Weight fraction of chemical in product (unitless)

CF $\quad=\quad$ Conversion factor (1000 mg/g)

f $\quad=\quad$ Fraction of mass emitted from first exponential (0.1) (unitless)

t_{start} $\quad=\quad$ Time of start of application (min)

t_a $\quad=\quad$ Application time (min)

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

t $\quad=\quad$ Time (min)

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

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

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

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, 1996). 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.

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

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).

$$ER_1(t) = \frac{M \times WF \times CF \times f}{t_a} \times [1 - H(t)]$$ (18)

Where:

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

M =   Mass of product used (g)

WF =   Weight fraction of chemical in product (unitless)

CF =   Conversion factor (1000 mg/g)

f =   Fraction of product emitted to air (unitless)

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

$$ER_2(t) = \frac{M \times WF \times CF}{t_a} \times \left[\left(1 - e^{-k(t - t_{start})}\right) - \left(\left(1 - e^{-k(t - (t_{start} + t_a))}\right) \times H(t) \right) \right]$$ (19)

Where:

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

M =   Mass of product used (g)

WF =   Weight fraction of chemical in product (unitless)

CF =   Conversion factor (1000 mg/g)

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

t_a =   Application time (min)

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

t =   Time (min)

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

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

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

$$ER_{final}(t) = ER_1(t) + ER_2(t) \tag{20}$$

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)

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

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% evaporation time.

$$EvapTime = \frac{145}{(MW \times VP)^{0.9546}} \times 60 \tag{21}$$

Where:

$EvapTime$ =   Evaporation time (min)

MW =   Molecular weight (g/mol)

VP =   Vapor pressure (Torr)

$$ER(t) = \frac{M \times WF \times CF}{EvapTime} \times H(t) \tag{22}$$

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)

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

Model assumes emission at a constant rate over a duration that depends on its molecular weight and vapor pressure, as shown in Equations 21 and 22. 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.

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:

$$LADC = \frac{C_{ati} \times FQ \times ED}{AT \times CF_1} \tag{23}$$

Where:

$LADC$ =   Potential Lifetime Average Daily Concentration (mg/m³-day)

C_{ati} =   Time-integrated air concentration for an event (mg/m³-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:

$$C_{ati} = \sum_{ST}^{ET} C_{i.t} \times \Delta t \tag{24}$$

Where:

C_{ati} =   Time-integrated, air concentration for an event (mg/m³-event) from start time (ST) to end time (ET), where ET = ST + 60 days.

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

Δt =   Time interval (3.47×10^{-4} days/event)

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

Peak concentration is the highest concentration experienced at any point during the day of use in the use environment. 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.

$$C_p = Max[\![C_{i,t}]\!]_{ST}^{ET}$$ (25)

Where:

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

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

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:

$$CADD = \frac{C_{air} \times Inh \times FQ \times D_{cr} \times ED}{BW \times AT \times CF_1 \times CF_2}$$ (26)

Where:

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

C_{air} =   Concentration of chemical in air (mg/m³)

Inh =   Inhalation rate (m³/hr)

FQ =   Frequency of use (events/year)

D_{cr} =   Duration of use (min/event), chronic

ED =   Exposure duration (years of product usage)

BW =   Body weight (kg)

AT =   Averaging time (years)

CF_1 =   Conversion factor (365 days/year)

CF_2 =   Conversion factor (60 min/hr)

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 (m³/hr)[a]	Inhalation Rate After Use (m³/hr)[b]
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

[a]Table 6-2, light intensity values (EPA, 2011)
[b]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:

$$CADD = \frac{Dose_{ati} \times FQ \times ED}{BW \times AT \times CF_1}$$ (27)

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:

$$Dose_{ati} = \sum_{ST}^{ET} C_{i.t} \times \Delta t \times Inh_{i,t} \times CF_2$$ (28)

Where:

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

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

$Inh_{i,t}$ = Inhalation Rate for Zone i at time t (m³/hr)

Δt = Time interval (1.16 x 10⁻⁴ days/event)

CF_2 = Conversion factor (24 hs/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.

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:

$$ADR = \frac{C_{air} \times Inh \times FQ \times D_{ac} \times ED}{BW \times AT \times CF_1} \quad (29)$$

Where:

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

C_{air} = Concentration of chemical in air (mg/m³)

Inh = Inhalation rate (m³/hr)

FQ = Frequency of product use (events/day)

D_{ac} = Duration of use (min/event), acute

ED = Exposure duration (days of product usage)

BW = Body weight (kg)

AT = Averaging time (days)

CF_1 = Conversion factor (60 min/hr)

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$_{ati}$ is used:

$$Dose_{ati} = \sum_{ST}^{ET} C_{i,t} \times \Delta t \times Inh_{i,t} \times CF_2 \tag{30}$$

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^3)
$Inh_{i,t}$	=	Inhalation Rate for Zone i at time t (m^3/hr)
Δt	=	Time interval (1.16 x 10^{-4} days/event)
CF_2	=	Conversion factor (24 hrs/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.

CEM provides the ADR, Peak Concentration (mg/m^3), and Peak Dose (mg/day) in the reports. Peak Dose is calculated by multiplying the ADR by the receptor body weight.

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.
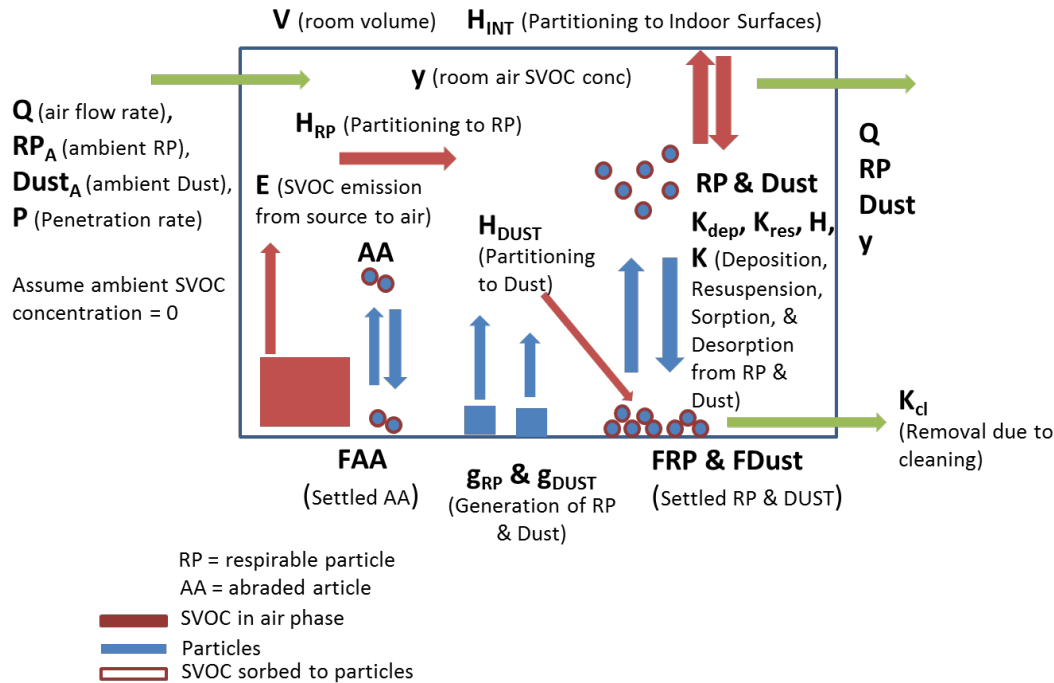
Figure 4. Schematic of fate and transport of SVOC in indoor environment

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 µm – 100 µm in diameter, referred to as "dust"); and fine particulates (10 µm in diameter or smaller, referred to as 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 µm), as well as incidental ingestion of SVOCs partitioned to settled dust. As such, while the model treats these entities separately based on mechanistic behavior, the values are combined as appropriate to estimate exposure as described in Appendix A. SVOC exposure can also occur via direct contact with articles, 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
Physical Parameters		
V	Volume of the room	m^3
Q	Ventilation rate of the room	m^3/hr
As	Area of emitting article surface	m^2
L_{Art}	Thickness of emitting article surface	m
ρ_{Art}	Density of emitting article	mg/m^3
$kdep_{RP}$	RP deposition rate constant	1/hr
$kdep_{Dust}$	Dust deposition rate constant	1/hr
$kdep_{AbArt}$	Abraded article particle deposition rate constant	1/hr
$kres_{RP}$	RP resuspension rate constant	1/hr

Symbol	Property	Units
$kres_{Dust}$	Dust resuspension rate constant	1/hr
$kres_{AbArt}$	Abraded article particle resuspension rate constant	1/hr
g_{abr}	Mass generation rate of abraded article particles	mg/hr
g_{ARP}	Mass generation rate of RP into indoor air	mg/hr
g_{ADust}	Mass generation rate of dust into indoor air	mg/hr
g_{FRP}	Mass generation rate of RP onto indoor floor	mg/hr
g_{FDust}	Mass generation rate of dust onto indoor floor	mg/hr
AmbRPConc	Concentration of RP in ambient air	mg/m^3
FilterPen	Air Filter Penetration Ratio	None
Clpr	Cleaning Periodicity	1/hr
cl_{eff}	Cleaning Efficiency	None
$k_{cl}(t)$	Binary switch representing whether cleaning is ongoing (based on Clpr)	None
$Z(t)$	Binary switch representing whether product is present in room	None
ρ_{RP}	Density of RP particle	mg/m^3
ρ_{Dust}	Density of dust particle	mg/m^3
r_{RP}	Radius of RP particle	m
r_{Dust}	Radius of dust particle	m
r_{AbArt}	Radius of abraded article particles	m
A_{Int}	Area of interior surfaces	m^2
L_{Int}	Thickness of sorbing portion of interior surfaces	m
Chemical Parameters		
h	SVOC gas phase mass transfer coefficient	m/hr
K_{RP}	SVOC RP-air partition coefficient	m^3/mg
K_{Dust}	SVOC dust-air partition coefficient	m^3/mg
K_{Art}	SVOC article-air partition coefficient	None
K_{Int}	SVOC -air partition coefficient	None
H_{RP}	RP 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^3
Inventory Terms		
N_{air}	SVOC mass in the gas phase in air	µg
N_{ARP}	SVOC mass sorbed to suspended RP in the air	µg
N_{ADust}	SVOC mass sorbed to suspended dust in the air	µg
N_{FRP}	SVOC mass sorbed to settled RP 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_{RP}	Mass of RP 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_{RP}	Mass of RP 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

[a]The thickness of emitting article surface value can impact emissions. EPA is considering article-specific thicknesses.

Default model inputs are provided in Table B-15. 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).

$$A_{int} = 2.08 \times V \tag{31}$$

Where:

A_{Int} = Area of Interior Surfaces (m^2)

V = Volume of Room (m^3)

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

$$
\begin{aligned}
\frac{dN_{Air}}{dt} =\ & Z(t) \times h \times A_s \times \frac{C_{0Art}}{K_{Art}} \times e^{-\left(\frac{h}{K_{Art} \times L_{Art}} \times t\right)} \\
& - \frac{Q}{V} \times N_{air} \\
& - H_{RP} \times \frac{A_{RP}}{\rho_{RP}} \times \frac{3}{r_{RP}} \times \left(\frac{N_{air}}{V} - \frac{N_{ARP}}{A_{RP}} \times \frac{1.0}{K_{RP}}\right) \\
& - H_{Dust} \times \frac{A_{Dust}}{\rho_{Dust}} \times \frac{3}{r_{Dust}} \times \left(\frac{N_{air}}{V} - \frac{N_{ADust}}{A_{Dust}} \times \frac{1.0}{K_{Dust}}\right) \\
& - H_{RP} \times \frac{F_{RP}}{\rho_{RP}} \times \frac{1.5}{r_{RP}} \times \left(\frac{N_{air}}{V} - \frac{N_{FRP}}{F_{RP}} \times \frac{1.0}{K_{RP}}\right) \\
& - H_{Dust} \times \frac{F_{Dust}}{\rho_{Dust}} \times \frac{1.5}{r_{Dust}} \times \left(\frac{N_{air}}{V} - \frac{N_{FDust}}{F_{Dust}} \times \frac{1.0}{K_{Dust}}\right) \\
& - H_{Int} \times \left(\frac{N_{air}}{V} - \frac{N_{Int}}{A_{Int} \times L_{Int}} \times \frac{1.0}{K_{Int}}\right) \times A_{Int} \\
& - H_{AbArt} \times \frac{A_{AbArt}}{\rho_{Art}} \times \frac{3}{r_{AbArt}} \times \left(\frac{N_{air}}{V} - \frac{N_{A\_AbArt}}{A_{AbArt}} \times \frac{\rho_{Art}}{K_{Art}}\right) \\
& - H_{AbArt} \times \frac{F_{AbArt}}{\rho_{Art}} \times \frac{1.5}{r_{AbArt}} \times \left(\frac{N_{air}}{V} - \frac{N_{F\_AbArt}}{F_{AbArt}} \times \frac{\rho_{Art}}{K_{Art}}\right)
\end{aligned}
\tag{32}
$$

Mass Balance for SVOC Sorbed to Suspended RP

$$\frac{d_{N_{ARP}}}{dt} = H_{RP} \times \frac{A_{RP}}{\rho_{RP}} \times \frac{3}{r_{RP}} \times \left(\frac{N_{air}}{V} - \frac{N_{ARP}}{A_{RP}} \times \frac{1.0}{K_{RP}}\right)$$
$$+ kres_{RP} \times N_{FRP} - kdep_{RP} \times N_{ARP} - \frac{Q}{V} \times N_{ARP}$$

(33)

Mass Balance for SVOC Sorbed to Suspended Dust

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

(34)

Mass Balance for SVOC Sorbed to Settled RP

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

(35)

Mass Balance for SVOC Sorbed to Settled Dust

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

(36)

Mass Balance for SVOC Sorbed to Interior Surfaces (Sinks)

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

(37)

Mass Balance for Suspended RP

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

(38)

Mass Balance for Suspended Dust

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

(39)

Mass Balance for Settled RP

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

(40)

Mass Balance for Settled Dust

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

(41)

Mass Balance for SVOC in Suspended Abraded Article Particles

$$\frac{dN_{A\_AbArt}}{dt} = g_{abr} \div \rho_{Art} \times C_{0\,Art} \times e^{-(\frac{h}{K_{Art} \times L_{Art}} \times t)}$$

$$+ H_{AbArt} \times \frac{A_{AbArt}}{\rho_{Art}} \times \frac{3}{r_{AbArt}} \times (\frac{N_{air}}{V} - \frac{N_{A\_AbArt}}{A_{AbArt}} \times \frac{\rho_{Art}}{K_{Art}})$$

$$+ kres_{AbArt} \times N_{F\_AbArt}$$

$$- kdep_{AbArt} \times N_{A\_AbArt}$$

$$- \frac{Q}{V} \times N_{A\_AbArt}$$

(42)

Mass Balance for SVOC in Settled Abraded Article Particles

$$\frac{dN_{F\_AbArt}}{dt} = + H_{AbArt} \times \frac{F_{AbArt}}{\rho_{Art}} \times \frac{1.5}{r_{AbArt}} \times (\frac{N_{air}}{V} - \frac{N_{F\_AbArt}}{F_{AbArt}} \times \frac{\rho_{Art}}{K_{Art}})$$

$$- kres_{AbArt} \times N_{F\_AbArt}$$

$$+ kdep_{AbArt} \times N_{A\_AbArt}$$

$$- k_{cl}(t) \times Cl_{eff} \times N_{F\_AbArt}$$

(43)

Mass Balance for Suspended Abraded Article Particles

$$\frac{dA_{AbArt}}{dt} = g_{abr}$$

$$+ kres_{AbArt} \times F_{AbArt}$$

$$- kdep_{AbArt} \times A_{AbArt}$$

$$- \frac{Q}{V} \times A_{AbArt}$$

(44)

Mass Balance for Settled Abraded Article Particles

$$\frac{dF_{AbArt}}{dt} = - kres_{AbArt} \times F_{AbArt}$$

$$+ kdep_{AbArt} \times A_{AbArt}$$

$$- k_{cl}(t) \times Cl_{eff} \times F_{AbArt}$$

(45)

Note: In Equations 33, 34, and 42, the value of 3/r is used to describe the surface area to volume ratio of a sphere. In Equations 35, 36, and 43, the value of 1.5/r indicates that for settled particles, only half of the surface area is available for mass transfer.

A series of terms from the mass balance calculations are required for calculating dose. The following equations (46-55) present the outputs from the mass balance equations that are used in the dose equations.

$$C_{gas} = \frac{N_{air}}{V} \tag{46}$$

$$SVOC_{RP\_air} = \frac{N_{ARP}}{V} \tag{47}$$

$$SVOC_{Dust\_air} = \frac{N_{ADust}}{V} \tag{48}$$

$$SVOC_{AbArt\_air} = \frac{N_{A\_AbArt}}{V} \tag{49}$$

$$Dust_{air} = \frac{A_{RP}}{V} \tag{50}$$

$$RP_{air} = \frac{A_{Dust}}{V} \tag{51}$$

$$AbArt_{air} = \frac{A_{AbArt}}{V} \tag{52}$$

$$SVOCfloor_{RP} = \frac{N_{FRP}}{F_{RP}} \tag{53}$$

$$SVOCfloor_{Dust} = \frac{N_{Dust}}{F_{Dust}} \tag{54}$$

$$SVOCfloor_{AbArt} = \frac{N_{AbArt}}{F_{AbArt}} \tag{55}$$

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:

$$h = 46.8 \times \frac{3.3}{\left(2.5 + MW^{1/3}\right)^2} \tag{56}$$

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 56) 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/m³) can be estimated using the following general equation, where 'part' refers to either RP or Dust as appropriate (Little et al., 2012):

$$K_p = f_{om\_part} \times \frac{K_{oa}}{\rho_{part}} \tag{57}$$

Where:

K_p = SVOC partition coefficient for RP (K_{RP}) or dust (K_{Dust}) (m³/mg)

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

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

ρ_{part} = Density of airborne particles; suggested value 1 x 10⁹ (mg/m³)

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):

$$\ln(K_{solid}) = 8.86 - 0.785 \times \ln(V_p) \tag{58}$$

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}

$$D_S = \frac{3 \times 10^{-11}}{(MW \div 292)^{6.5}} \tag{59}$$

Where:

D_S = Solid-phase diffusion coefficient (m²/hr)

MW = Molecular weight (g/mol)

$$K_{solid} = e^{(8.86 - 0.785 \times ln(VP))} \tag{60}$$

Where:

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

VP =   Vapor pressure (Torr)

$$h_a = 46.8 \times (3.3 \div (2.5 + MW^{\frac{1}{3}})^2 \tag{61}$$

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):

$$\frac{1}{H_{solid}} = \frac{1}{h_a} + \frac{1}{\frac{2D_s}{L}K_{solid}} \tag{62}$$

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 (61)

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:

$$\left(\frac{D_0}{D_1}\right) = \left(\frac{MW_1}{MW_0}\right)^{6.5} \tag{63}$$

Where:

D_0 =   3×10^{-11} (m^2/hr) is the diffusion coefficient for the reference compound (PCB-52)

D_1 =   Diffusion coefficient for compound of interest (m^2/hr)

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 partitioning and diffusion coefficients are presented in Tables B-17 and B-18, respectively. 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 CADD and the Potential ADR. Both gas-phase and airborne RP-bound SVOCs are assumed to be available for inhalation. The general expression for the Potential CADD is as follows:

$$CADD_{Air} = \frac{C_{gas\_avg} \times FracTime \times InhalAfter \times CF_1}{BW \times CF_2} \tag{64}$$

$$CADD_{Particulate} = \frac{SVOCRP_{air\_avg} \times RP_{air\_avg} \times (1 - IF_{RP}) FracTime \times InhalAfter \times CF_1}{BW \times CF_2} \tag{65}$$

$$CADD_{total} = CADD_{Air} + CADD_{Particulate} \tag{66}$$

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 (µg/m³)
$SVOCRP_{air\_avg}$	=	Average SVOC in RP concentration, air (µg/mg)
RP_{air_avg}	=	Average RP concentration, air (mg/m³)
IF_{RP}	=	RP ingestion fraction (unitless)
$FracTime$	=	Fraction of time in environment (unitless)
$InhalAfter$	=	Inhalation rate after use (m³/hr)
CF_1	=	Conversion factor (24 hrs/day)
BW	=	Body weight (kg)
CF_2	=	Conversion factor (1000 µg/mg)

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

$$ADR_{Air} = \frac{C_{gas\_max} \times FracTime \times InhalAfter \times CF_1}{BW \times CF_2} \tag{67}$$

$$ADR_{Particulate} = \frac{SVOCRP_{air\_max} \times RP_{air\_avg} \times FracTime \times InhalAfter \times CF_1}{BW \times CF_2} \tag{68}$$

$$ADR_{total} = ADR_{Air} + ADR_{Particulate} \tag{69}$$

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 (µg/m³)
$SVOCRP_{air\_max}$	=	Maximum SVOC in RP concentration, air (µg/mg)
RP_{air_max}	=	Maximum RP concentration, air (mg/m³)
$FracTime$	=	Fraction of time in environment (unitless)
$InhalAfter$	=	Inhalation rate after use (m³/hr)
CF_1	=	Conversion factor (24 hrs/day)
BW	=	Body weight (kg)
CF_2	=	Conversion factor (1000 µg/mg)

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).

$$CADD = \frac{FQ_{cr} \times M \times WF \times F_{ing} \times CF_1 \times ED_{cr}}{BW \times AT_{cr} \times CF_2} \qquad (70)$$

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)
CF_1	=	Conversion factor (1000 mg/g)
ED_{cr}	=	Exposure duration, chronic (years)
BW	=	Body weight (kg)
AT_{cr}	=	Averaging time, chronic (years), 78 years for LADD
CF_2	=	Conversion factor (365 days/year)

$$ADR = \frac{FQ_{ac} \times M \times WF \times F_{ing} \times CF_1 \times ED_{ac}}{BW \times AT_{ac}} \qquad (71)$$

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)

CF_1 =   Conversion factor (1000 mg/g)

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

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

BW =   Body weight (kg)

P_ING2: Ingestion of Product Applied to Ground Outdoors

Model assumes ingestion of chemical mixed with soil particles after the product, such as fertilizer, is applied directly to the ground. The model divides the mass of chemical (mass of product multiplied by weight fraction of chemical) by the volume of soil (area of application multiplied by the soil mixing depth, density, and porosity) to get the concentration in the soil. Chemical decay and physical transport away from the surface soil, as well as repeat applications, are accounted for in the frequency and soil half-life terms. As currently incorporated, the CADD reports the average dose over 1 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).

$$CADD = \frac{M \times WF \times Freq \times D \times \left(\frac{1}{365ln(2)/t_{1/2}}\right) \times \left(1-e^{-\left(\frac{365ln(2)}{t_{1/2}}\right)}\right) \times SoilIng \times ED_{cr} \times CF_1}{Area \times Depth \times \rho \times (1-\emptyset) \times AT_{cr} \times BW} \quad (72)$$

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)

$Freq$ =   Frequency of use/application (use/year)

D =   Duration of application (1 year)

$t_{1/2}$ =   Chemical half-life in soil (days)

$SoilIng$ =   Incidental soil ingestion rate (mg/day)

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

CF_1 =   Conversion factor (1 kg/1000 g)

$Area$ =   Area of yard product is applied (m^2)

$Depth$ =   Soil mixing depth (m)

ρ =   Soil density (kg/m^3)

$\emptyset$ = Soil porosity (unitless)

AT_{cr} = Averaging time, chronic (years), 78 years for lifetime

BW = Body weight (kg)

$$ADR = \frac{M \times WF \times Freq \times D \times \left(\frac{1}{\ln(2)/t_{1/2}}\right) \times \left(1 - e^{-\left(\frac{\ln(2)}{t_{1/2}}\right)}\right) \times SoilIng \times ED_{cr} \times CF_1}{Area \times Depth \times \rho \times (1 - \emptyset) \times AT_{cr} \times BW} \tag{73}$$

Where:

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

M = Mass of product used (g)

WF = Weight fraction of chemical in product (unitless)

$Freq$ = Frequency of use/application (use/day)

D = Duration of application (1 day)

$t_{1/2}$ = Chemical half-life in soil (days)

$SoilIng$ = Incidental soil ingestion rate (mg/day)

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

CF_1 = Conversion factor (1 kg/1000 g)

$Area$ = Area of yard product is applied (m^2)

$Depth$ = Soil mixing depth (m)

ρ = Soil density (kg/m^3)

$\emptyset$ = Soil porosity (unitless)

AT_{ac} = 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 4** based on K$_p$, soil and standard biodegradation test results (ECHA, 2016). For K$_p$ 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)

Kp, soil	Readily biodegradable	Readily biodegradable, failing 10-d window	Inherently biodegradable
<100	30	90	300
>100, <1000	300	900	3,000
>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.

$$CADD_{IAI} = \frac{\left[(SVOCRP_{air\_avg} \times RP_{air_{avg}} \times IF_{RP}) + (SVOCDust_{air\_avg} \times Dust_{air_{avg}} \times IF_{Dust}) + (SVOCAbr_{air\_avg} \times Abr_{air\_avg} \times IF_{Abr})\right] \times InhalAfter \times CF_1}{BW \times CF_2}$$

(74)

Where:

$CADD_{IAI}$	=	Potential Chronic Average Daily Dose from ingestion after inhalation (mg/kg-day)
$SVOCRP_{air\_avg}$	=	Average SVOC in RP concentration, air (µg/mg)
RP_{air_avg}	=	Average RP concentration, air (mg/m³)
IF_{RP}	=	RP ingestion fraction (unitless)
$SVOCDust_{air\_avg}$	=	Average SVOC dust concentration, air (µg/mg)
$Dust_{air\_avg}$	=	Average dust concentration, air (mg/m³)
IF_{Dust}	=	Dust ingestion fraction (unitless)
$SVOCAbr_{air\_avg}$	=	Average SVOC in abraded particle concentration, air (µg/mg)
Abr_{air_avg}	=	Average abraded particle concentration, air (mg/m³)
IF_{Abr}	=	Abraded particle ingestion fraction (unitless)
$InhalAfter$	=	Inhalation rate after use (m³/hr)
CF_1	=	Conversion factor (24 hrs/day)
BW	=	Body weight (kg)
CF_2	=	Conversion factor (1000 mg/g)

$$ADR_{IAI} = \frac{\left[(SVOCRP_{air\_max} \times RP_{air\_max} \times IF_{RP}) + (SVOCDust_{air\_max} \times Dust_{air\_max} \times IF_{Dust}) + (SVOCAbr_{air\_max} \times Abr_{air\_max} \times IF_{Abr})\right] \times InhalAfter \times}{BW \times CF_2}$$

(75)

Where:

ADR_{IAI}	=	Potential Acute Dose Rate from Ingestion and Inhalation (mg/kg-day)
$SVOCRP_{air\_max}$	=	Maximum SVOC in RP concentration, air (µg/mg)
RP_{air_max}	=	Maximum RP concentration, air (mg/m³)

IF_{TSP}	=	RP ingestion fraction (unitless)
$SVOCDust_{air\_max}$	=	Maximum SVOC in dust concentration, air (µg/mg)
$Dust_{air\_max}$	=	Maximum dust concentration, air (mg/m^3)
IF_{Dust}	=	Dust ingestion fraction (unitless)
$SVOCAbr_{air\_avg}$	=	Maximum SVOC in abraded particle concentration, air (µg/mg)
Abr_{air_avg}	=	Maximum abraded particle concentration, air (mg/m^3)
IF_{Abr}	=	Abraded particle ingestion fraction (unitless)
$InhalAfter$	=	Inhalation rate after use (m^3/hr)
CF_1	=	Conversion factor (24 hrs/day)
BW	=	Body weight (kg)
CF_2	=	Conversion factor (1000 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).

$$CADD = \frac{MR \times CA \times D_m \times ED_{cr} \times CF_1}{BW \times AT_{cr} \times CF_2} \tag{76}$$

Where:

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

$$ADR = \frac{MR \times CA \times D_m \times ED_{ac} \times CF_1}{BW \times AT_{ac} \times CF_2} \tag{77}$$

Where:

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

MR = Migration rate of chemical from article to saliva (mg/cm^2/hr)

CA = Contact area of mouthing (cm^2)

D_m = Duration of mouthing (min/hr)

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

CF_1 = Conversion factor (24 hrs/day)

BW = Body weight (kg)

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

= Conversion factor (60 min/hr)

The migration rate of the chemical from the article to saliva is a user defined input that is used in Equations 76 and 77 to calculate the dose from ingestion of an article mouthed. CEM provides guidance (**Table 5**) as to what value should be used, but there is no estimator equation. The migration rate suggestions depend on the concentration range and are independent of the chemical's physicochemical properties. This means that the dose resulting from ingestion of an article mouthed will not scale with the amount of chemical used. Using an extremely low chemical weight fraction also requires using a correspondingly low migration rate.

Table 5. Suggested migration rates based on chemical concentration

Migration Rate	Concentration Range
10 mg/cm^2/hr	>10,000 ppm
0.1 mg/cm^2/hr	100-10,000 ppm
1 x 10^{-3} mg/cm^2/hr	1- 100 ppm
1 x 10^{-4} mg/cm^2/hr	<1 ppm

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. The model uses a weighted dust concentration, shown in Equations 78 and 79 for acute and chronic, respectively.

$$Dust_{cr\_wgt} = \frac{(RP_{floor\_avg} \times SVOCRP_{floor\_avg}) + (Dust_{floor\_avg} \times SVOCDust_{floor\_avg}) + (AbArt_{floor\_avg} \times SVOCAbArt_{floor\_avg})}{(RP_{floor\_avg} + Dust_{floor\_avg} + AbArt_{floor\_avg})} \quad (78)$$

Where:

$Dust_{cr\_wgt}$ = Chronic weighted dust concentration (µg/mg)

RP_{floor_avg} = Average RP mass, floor (mg)

$SVOCRP_{floor\_avg}$ = Average SVOC in RP concentration, floor (µg/mg)

$Dust_{floor\_avg}$ = Average dust mass, floor (mg)

$SVOCDust_{floor\_avg}$ =   Average SVOC in dust concentration, floor (µg/mg)

$AbArt_{floor\_avg}$ =   Average abraded particles mass, floor (mg)

$SVOCAbArt_{floor\_avg}$ =   Average floor dust SVOC concentration (µg/mg)

$$Dust_{ac\_wgt} = \frac{(RP_{floor\_max} \times SVOCRP_{floor\_max}) + (Dust_{floor\_max} \times SVOCDust_{floor\_max}) + (AbArt_{floor\_max} \times SVOCAbArt_{floor\_max})}{(TSP_{floor\_max} + Dust_{floor\_max} + AbArt_{floor\_max})} \tag{79}$$

Where:

$Dust_{ac\_wgt}$ =   Acute weighted dust concentration (µg/mg)

RP_{floor_max} =   Maximum RP mass, floor (mg)

$SVOCRP_{floor\_max}$ =   Maximum SVOC in RP concentration, floor (µg/mg)

$Dust_{floor\_max}$ =   Maximum dust mass, floor (mg)

$SVOCDust_{floor\_max}$ =   Maximum SVOC in dust concentration, floor (µg/mg)

$AbArt_{floor\_max}$ =   Maximum abraded particles mass, floor (mg)

$SVOCAbArt_{floor\_max}$ =   Maximum floor dust SVOC concentration (µg/mg)

$$CADD = \frac{Dust_{cr\_wgt} \times FracTime \times DustIng}{BW \times CF} \tag{80}$$

Where:

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

$Dust_{cr\_wgt}$ =   Chronic weighted dust concentration (µg/mg)

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

$DustIng$ =   Dust ingestion rate (mg/day)

BW =   Body weight (kg)

CF =   Conversion factor (1000 µg/mg)

$$ADR = \frac{Dust_{ac\_wgt} \times FracTime \times DustIng}{BW \times CF} \tag{81}$$

Where:

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

$Dust_{ac\_wgt}$ =   Acute weighted dust concentration (µg/mg)

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

$DustIng$ =   Dust ingestion rate (mg/day)

BW = Body weight (kg)

CF = Conversion factor (1000 µg/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.

$$C_d = \frac{C_{0\_art} \times K_{dust} \times CF}{K_{solid}}$$ (82)

Where:

C_d = Concentration of SVOC in dust (mg/mg)

C_{0_art} = Initial SVOC concentration in article (mg/cm³)

K_{dust} = SVOC dust-air partition coefficient (m³/mg)

CF = Conversion factor (10^6 cm³/m³)

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

Once the SVOC concentration in the dust is estimated, the acute dose rate can be calculated. In this scenario, there is no difference between chronic and acute exposure, as both would rely on the same upper end dust concentration.

$$ADR_{DTD} = \frac{C_d \times FracTime \times DustIng}{BW}$$ (83)

Where:

ADR_{DTD} = Potential Acute Dose Rate from direct transfer to dust (mg/kg-day)

C_d = Concentration of SVOC in dust (mg/mg)

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

$DustIng$ = Dust ingestion rate (mg/day)

BW = Body weight (kg)

P_DER1: Dermal Dose from Direct Transfer from Vapor Phase to Skin

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):

$$K_{p\_cw} = 10^{(0.7 \times LogK_{ow} - 0.0722 \times MW^{\frac{2}{3}} - 5.252)} \tag{84}$$

$$K_{p\_w} = \frac{K_{p\_cw}}{1 + (K_{p\_cw} \times MW^{0.5})/2.6} \tag{85}$$

$$K_{p\_b} = \frac{K_{p\_w}}{40.9 \times H} \tag{86}$$

$$K_{p\_g} = \left(\frac{1}{V_d} + \frac{1}{K_{p\_b}}\right)^{-1} \tag{87}$$

Where:

K_{p_cw} =   Permeability coefficient through stratum corneum of a chemical when the species concentration is measured in water in contract with skin (m/hr)

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 a chemical when the species concentration is measured in water in contact with skin (m/hr)

K_{p_b} =   Permeability coefficient that describes the transport of a gas-phase chemical from the boundary layer at the skin surface (b) through the stratum corneum/viable epidermis composite to dermal capillaries (m/hr)

H =   Henry's law coefficient (atm/M)

K_{p_g} =   Indoor air transdermal permeability coefficient that describes transport of a gas-phase chemical 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/hr)

V_d =   Deposition velocity (m/hr)

Because the concentration varies between Zone 1 and Zone 2, and the receptor can be present in either room, it is necessary to calculate the flux that would occur in each of the zones as well as the time spent in each of the zones, as shown in the following calculations.

$$DerFlux_{z1,c} = \frac{K_{p\_g} \times C_{g,z1c}}{CF} \tag{88}$$

$$DerFlux_{z2,c} = \frac{K_{p\_g} \times C_{g,z2c}}{CF} \tag{89}$$

Where:

$DerFlux_{z1,c}$ =   Chronic dermal flux in Zone 1 (µg/cm²-hr)

$DerFlux_{z2,c}$ =   Chronic dermal flux in Zone 2 (µg/cm²-hr)

K_{p_g} =   Transdermal permeability coefficient (m/hr)

$C_{g,z1c}$ =   Average chronic gas phase concentration for Zone 1 (µg/cm³)

$C_{g,z2c}$ =   Average chronic gas phase concentration for Zone 2 (µg/cm³)

CF =   Conversion factor (10,000 cm²/m²)

$$\log(K_{l\_g}) = 0.74 + \log(K_{ow}) + \log(H) + \log(RT) \tag{90}$$

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)

$$CADD = \frac{\left(DerFlux_{z1,c} \times \text{FracTime}_{z1,c} + DerFlux_{z2,c} \times \text{FracTime}_{z2,c}\right) \times \frac{SA}{BW} \times ED_{cr} \times CF_1}{AT_{cr} \times CF_2}$$

$$\tag{91}$$

Where:

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

$DerFlux_{z1,c}$ =   Chronic dermal flux for Zone 1 (µg/cm²-hr)

$\text{FracTime}_{z1,c}$ =   Fraction of time in Zone 1 during one year (unitless)

$DerFlux_{z2,c}$ =   Chronic dermal flux for Zone 2 (µg/cm²-hr)

$\text{FracTime}_{z2,c}$ =   Fraction of time in Zone 2 during one year (unitless)

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

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

CF_1 =   Conversion factor (24 hrs/day)

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

CF_2 =   Conversion factor (1000 µg/mg)

$$DerFlux_{z1,a} = \frac{K_{p\_g} \times C_{g,z1a}}{CF} \tag{92}$$

$$DerFlux_{z2,a} = \frac{K_{p\_g} \times C_{g,z2a}}{CF} \tag{93}$$

Where:

$DerFlux_{z1,a}$ =   Dermal flux for Zone 1 (µg/cm²-hr)

$DerFlux_{z2,a}$ =   Dermal flux for Zone 2 (µg/cm²-hr)

K_{p_g} =   Transdermal permeability coefficient (m/hr)

$C_{g,z1a}$ = Acute average gas phase concentration in Zone 1 ($\mu g/cm^3$)

$C_{g,z2a}$ = Acute average gas phase concentration in Zone 2 ($\mu g/cm^3$)

CF = Conversion factor (10,000 cm^2/m^2)

$$ADR = \frac{\left(DerFlux_{z1,a} \times \text{FracTime}_{z1,a} + DerFlux_{z2,a} \times \text{FracTime}_{z2,a}\right) \times \frac{SA}{BW} \times ED_{ac} \times CF_1}{AT_{ac} \times CF_2}$$

(94)

Where:

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

$DerFlux_{z1,a}$ = Dermal flux for Zone 1 ($\mu g/cm^2$-hr)

$\text{FracTime}_{z1,a}$ = Fraction of time in Zone 1 during one day (unitless)

$DerFlux_{z2,a}$ = Dermal flux for Zone 2 ($\mu g/cm^2$-hr)

$\text{FracTime}_{z2,a}$ = Fraction of time in Zone 2 during one day (unitless)

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

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

CF_1 = Conversion factor (24 hrs/day)

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

CF_2 = Conversion factor (1,000 $\mu g/mg$)

CEM includes six prepopulated generic product scenarios that include this model. They are listed in the existing analyses as "Generic P1 E1 + VS" and there is one for each emission model.

Note, the user will need to consider what the appropriate the surface area to body weight ratio default value should be considering the specific scenario modeled. See Table B-3 in the Appendix for more guidance.

P_DER2a: 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^2-event) is the product of the film thickness of the liquid on the skin's surface and the density of the formulation.

$$AR = FT \times \rho \times (1 - \text{FracRemove})$$ (95)

Where:

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

FT = Film Thickness (cm)

ρ =   Density of formulation (g/cm^3)

$FracRemove$ =   Fraction of product removed by washing or wearing (unitless)

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

(96)

Where:

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

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

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

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

FR_{abs} =   Absorption fraction (unitless)

Dil =   Product dilution fraction (unitless)

WF =   Weight fraction of chemical in product (unitless)

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

CF_1 =   Conversion factor (1000 mg/g)

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

CF_2 =   Conversion factor (365 days/year)

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

(97)

Where:

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

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

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

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

FR_{abs} =   Absorption fraction (unitless)

Dil   =   Product dilution fraction (unitless)

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)

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):

$$FR_{abs} = \frac{3 + \chi\left[1 - \exp\left(-a\frac{D_{cr}}{t_{lag} \times CF_1}\right)\right]}{3(1+\chi)}$$

(98)

χ =   Ratio of the evaporation rate from the SC surface to the dermal absorption rate through the SC (unitless)

α =   Constant (2.906)

D_{cr} =   Duration of use (min)

t_{lag} =   Lag time for chemical transport through the SC (hr)

CF_1 =   Conversion factor (60 min/hr)

Where t$_{lag}$ is defined as:

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

(99)

h_{SC} =   Stratum corneum thickness (assumed to be 15 µm)

MW =   Molecular weight (mg/mmol)

Where χ is defined as:

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

(100)

h =   Gas phase mass transfer coefficient (m/hr)

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/hr)

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 100 is estimated using the built in CEM estimator from P_DER2b (Equation 101). The gas phase mass transfer coefficient (h) is estimated using Equation 56.

The user should take note that there is the potential for this model methods overestimate the dermal absorption, as the product mass does not explicitly enter the model equations.

Note, the user will need to consider what the appropriate the surface area to body weight ratio default value should be considering the specific scenario modeled. See Table B-3 in the Appendix for more guidance.

P_DER2b: 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:

1. Entering a permeability coefficient
2. Using the "Estimate" button and having the model calculate the permeability coefficient using the following equation (ten Berge, 2010):

$$K_p = \frac{1}{\left(\frac{1}{K_{lip}+K_{pol}}\right)+\left(\frac{1}{K_{aq}}\right)} \tag{101}$$

Where,

K_p =   Permeability coefficient for chemical transport through the SC from an aqueous vehicle (cm/hr)

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 102-104, respectively,

$$K_{lip} = 10^{(-2.96+0.981 \times log(K_{ow})-0.0079 \times MW)} \tag{102}$$

$$K_{pol} = \frac{0.0552}{MW^{1.38}} \tag{103}$$

$$K_{aq} = \frac{1121}{MW^{1.96}} \tag{104}$$

$$CADD = \frac{K_p \times D_{cr} \times Dil \times \rho \times \frac{SA}{BW} \times FQ_{cr} \times WF \times ED_{cr} \times CF_1}{AT_{cr} \times CF_2 \times CF_3}$$ (105)

Where:

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

K_p = Permeability coefficient (cm/hr)

D_{cr} = Duration of use (min/event), chronic

Dil = Product dilution fraction (unitless)

ρ = Density of formulation (g/cm^3)

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

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

WF = Weight fraction of chemical in product (unitless)

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

CF_1 = Conversion factor (1000 mg/g)

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

CF_2 = Conversion factor (60 min/hr)

CF_3 = Conversion factor (365 days/year)

$$ADR = \frac{K_p \times D_{ac} \times Dil \times \rho \times \frac{SA}{BW} \times FQ_{ac} \times WF \times ED_{ac} \times CF_1}{AT_{ac} \times CF_2}$$ (106)

Where:

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

K_p = Permeability coefficient (cm/hr)

D_{ac} = Duration of use (min/event), acute

Dil = Product dilution fraction (unitless)

ρ = Density of formulation (g/cm^3)

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

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

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)

CF_2 = Conversion factor (60 min/hr)

The user should take note that there is the potential for this model methods overestimate the dermal absorption, as the product mass does not explicitly enter the model equations. For P_DER2b, it is possible that more chemical is absorbed than was originally present. The assumption that any chemical penetrating the skin is replaced by more from an unlimited source may need to be checked. Also, P_DER2b is effectively for "occluded" contact and will overestimate the absorption if the contact is intermittent.

Note, the user will need to consider what the appropriate the surface area to body weight ratio default value should be considering the specific scenario modeled. See Table B-3 in the Appendix for more guidance.

P_DER3: 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 107 and 108 estimate the concentration of a chemical in soil to be used in CADD and ADR:

$$C_{soil,cr} = \frac{M \times WF \times CF_m \times \left(\frac{1}{253/t_{1/2}}\right) \times \left(1 - e^{-\left(\frac{253}{t_{1/2}}\right)}\right)}{Area \times Depth \times \rho \times (1 - \emptyset)} \tag{107}$$

Where:

$C_{soil,cr}$ =   Concentration of chemical in soil (mg/kg), chronic

M   =   Mass of product used per application (g)

WF   =   Weight fraction (unitless)

CF_m =   Conversion factor (1000 mg/g)

$t_{1/2}$ =   Chemical half-life in soil

$Area$ =   Area of yard product is applied (m²)

$Depth$ =   Soil mixing depth (m)

ρ =   Soil density (kg/m³)

$\emptyset$ =   Soil porosity (unitless)

$$C_{soil,ac} = \frac{M \times WF \times CF_m \times \left(\frac{1}{0.69/t_{1/2}}\right) \times \left(1 - e^{-\left(\frac{0.69}{t_{1/2}}\right)}\right)}{Area \times Depth \times \rho \times (1 - \emptyset)} \tag{108}$$

Where:

$C_{soil,ac}$ =   Concentration of chemical in soil (mg/kg), acute

M   =   Mass of product used per application (g)

WF   =   Weight fraction (unitless)

CF_m =   Conversion factor (1000 mg/g)

$t_{1/2}$	=	Chemical half-life in soil
$Area$	=	Area of yard product is applied (m²)
$Depth$	=	Soil mixing depth (m)
ρ	=	Soil density (kg/m³)
$\emptyset$	=	Soil porosity (unitless)

$$CADD = \frac{C_{soil,cr} \times \frac{SA}{BW} \times AF \times FR_{abs} \times FQ_{cr} \times ED_{cr}}{CF_1 \times CF_2 \times AT_{cr}}$$ (109)

$CADD$	=	Potential Chronic Average Daily Dose (mg/kg-day)
$C_{soil,cr}$	=	Concentration in soil, dust or powder (mg/kg)
$\frac{SA}{BW}$	=	Surface area to body weight ratio (cm²/kg)
AF	=	Adherence factor of dust to hand (mg/cm²-event)
FR_{abs}	=	Fraction absorbed (unitless)
FQ_{cr}	=	Frequency of use (events/year)
ED_{cr}	=	Exposure duration, chronic (years)
CF_1	=	Conversion factor (1,000,000 mg/kg)
CF_2	=	Conversion factor (365 days/yr)
AT_{cr}	=	Averaging time, chronic (years)

$$ADR = \frac{C_{soil,ac} \times \frac{SA}{BW} \times AF \times FR_{abs} \times FQ_{ac} \times ED_{ac}}{CF_1 \times AT_{ac}}$$ (110)

ADR	=	Potential Acute Dose Rate (mg/kg-day)
$C_{soil,ac}$	=	Concentration in soil, dust, or powder (mg/kg)
$\frac{SA}{BW}$	=	Surface area to body weight ratio (cm²/kg)
AF	=	Adherence factor of soil or product to hand (mg/cm²-event)
FR_{abs}	=	Fraction absorbed (unitless)
FQ_{ac}	=	Events per day (events/day)
ED_{ac}	=	Exposure duration, acute (days)
CF_1	=	Conversion factor (1,000,000 mg/kg)
AT_{ac}	=	Averaging time, acute (days)

Note, the user will need to consider what the appropriate the surface area to body weight ratio default value should be considering the specific scenario modeled. See Table B-3 in the Appendix for more guidance.

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). This model is identical to P_DER1 with the exception that the calculations are based on a one zone, versus a two-zone model.

$$DerFlux = \frac{K_{p\_g} \times C_g}{CF} \tag{111}$$

Where:

$DerFlux$ = Dermal flux (µg/cm²-hr)

K_{p_g} = Transdermal permeability coefficient (m/hr)

C_g = Average gas phase concentration (µg/cm³)

CF = Conversion factor (100 cm/m)

$$\log(K_{l\_g}) = 0.74 + \log(K_{ow}) + \log(H) + \log(RT) \tag{112}$$

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)

$$CADD = \frac{DerFlux \times \frac{SA}{BW} \times \text{FracTime} \times ED_{cr} \times CF_1}{AT_{cr} \times CF_2} \tag{113}$$

Where:

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

$DerFlux$ = Dermal flux (µg/cm²-hr)

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

$$ADR = \frac{DerFlux \times \frac{SA}{BW} \times FracTime \times ED_{ac} \times CF_1}{AT_{ac} \times CF_2}$$ (114)

Where:

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

$DerFlux$ = Dermal flux (µg/cm²-hr)

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

FracTime = Fraction of time in environment (unitless)

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

CF_1 = Conversion factor (24 hrs/day)

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

CF_2 = Conversion factor (1000 µg/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. The model estimates dermal loading on the skin, or potential dose, rather than absorbed dose. Based on Delmaar et al. 2013, the average distance, *l*, a diffusing molecule will travel during contact, *Dur*, is calculated by the equation:

$$l = \left(\sqrt{2 \times (D \times 60) \times Dur} \right) \times CF_1$$ (115)

Where:

l = Average distance a diffusing molecule travels per contact (cm/day)

D = Solid phase diffusion coefficient (m²/hr)

D_{art} = Duration of article contact (min/day)

CF_1 = Conversion factor (100 cm/m)

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

$$CADD = \frac{C_{art} \times \frac{SA}{Bw} \times l \times FR_{abs\_art} \times ED_{cr}}{AT_{cr}}$$ (116)

Where:

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

C_{art} = Chemical concentration in article (mg/cm³)

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

FR_{abs_art} = Fraction absorbed (unitless)

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

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

$$ADR = \frac{C_{art} \times \frac{SA}{Bw} \times l \times FR_{abs\_art} \times ED_{ac}}{AT_{ac}}$$ (117)

Where:

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

C_{art} = Chemical concentration in article (mg/cm³)

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

FR_{abs_art} = Fraction absorbed (unitless)

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

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

Where fraction absorbed is calculated using Equation 118,

$$FR_{abs\_art} = \frac{3 + \chi \left[1 - \exp\left(-a \frac{D_{art}}{(EvD \times t_{lag} \times CF_1)} \right) \right]}{3(1+\chi)}$$ (118)

χ = Ratio of the evaporation rate from the SC surface to the dermal absorption rate through the SC (unitless)

α = Constant (2.906)

D_{art} = Duration of use (min/day)

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

t_{lag} = Lag time for chemical transport through the SC (hr)

CF_1 = Conversion factor (60 min/hr)

Where t_{lag} is calculated using Eq 99 and χ is calculated using Eq 100.

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 41). The CADD equation uses the average floor dust concentration, while for ADR the maximum floor dust concentration is used.

$$CADD = \frac{Dust_{cr\_wgt} \times \frac{SA}{BW} \times AF \times FA \times EvD \times ED_{cr}}{CF_1 \times AT_{cr}} \tag{119}$$

$CADD$	=	Potential Chronic Average Daily Dose (mg/kg-day)
$Dust_{cr\_wgt}$	=	Chronic weighted dust concentration (µg/mg)
$\frac{SA}{BW}$	=	Surface area to body weight ratio (cm^2/kg)
AF	=	Adherence factor of dust to hand (mg/cm^2-event)
FA	=	Fraction absorbed (unitless)
EvD	=	Frequency of article contact per day (events/day)
ED_{cr}	=	Exposure duration, chronic (years)
CF_1	=	Conversion factor (1000 µg/mg)
AT_{cr}	=	Averaging time, acute, chronic (years)

$$ADR = \frac{Dust_{ac\_wgt} \times \frac{SA}{BW} \times AF \times FA \times EvD \times ED_{ac}}{CF_1 \times AT_{ac}} \tag{120}$$

ADR	=	Potential Acute Dose Rate (mg/kg-day)
$Dust_{ac\_wgt}$	=	Acute weighted dust concentration (µg/mg)
$\frac{SA}{BW}$	=	Surface area to body weight ratio (cm^2/kg)
AF	=	Adherence factor of dust to hand (mg/cm^2-event)
FA	=	Fraction absorbed (unitless)
EvD	=	Frequency of article contact per day (events/day)
ED_{ac}	=	Exposure duration, acute (days)
CF_1	=	Conversion factor (1000 µg/mg)
AT_{ac}	=	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 considered.

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 $\mu g/m^3$). Applying a uniform value to "stop" an event across chemicals/scenarios such as 0.001 $\mu g/m^3$ or 1 ng/m^3 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 Bathing or Showering

An additional model may be added to CEM to model products added to water during a bath or shower. 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 121 and 122. 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.

$$CADD = \frac{K_p \times M \times D \times \frac{SA}{BW} \times FQ_{cr} \times ED_{cr} \times CF_1}{Q \times AT \times CF_2 \times CF_3} \qquad (121)$$

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^2)

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^3/gallons)

CF_3 = Conversion factor (365 days/yr)

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

$$FQ_{cr} = EV \times EF \tag{122}$$

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.

$$C = \left[\frac{M \times WF \times F \times N \times CF}{Q} \right] \times R \times SDF \tag{123}$$

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)

Q =   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 literature is emerging in this area and all exposure pathways are presented as potential in nature.

Products that Spill or Leak Over Time

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

Elevated Temperatures During Application and Use

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

Consideration of Multiple Zones in the SVOC Article Model

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

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

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

Consideration of Chemical or Material-Specific Migration Rates

Migration rates into saliva from sustained mouthing behavior are highly variable and understudied. EPA is aware of a few dozen studies that have quantified migration rates using units similar to $\mu g/cm^2/hr$. 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 be better characterize this important parameter. Factors that may influence the migration rate into saliva may include: size of chemical additive (molecular weight and/or molar volume); water solubility of chemical additive; chemical structure, concentration and/or loading of the chemical within the material; temperature (~37° C for human mouth), pH (~6.5 for human mouth), and composition (presences of salts, enzymes, etc.) of saliva or simulated saliva; and the type of material in contact with saliva or simulated saliva.

Consideration of Total Ingestion Rates of Indoor Dust and Particles

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

Consideration of Additional Exposure Scenarios and Exposure Defaults

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

Glossary

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

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.

Activity Pattern Description of where the receptor spends their time during a 24-hour day. CEM has three different activity patterns: stay-at-home, part-time out-of-the home (daycare, school, or work), and full-time out-of-the-home. The activity patterns were developed based on Consolidated Human Activity Database (CHAD).

Acute Dermal Flux in Zone 1; $DerFlux_{z1,a}$ (µg/cm²-hr) The rate of chemical flux from the air to the skin in Zone 1 resulting from product use in Zone 1 on the day of use.

Acute Dermal Flux in Zone 2; $DerFlux_{z2,a}$ (µg/cm²-hr) The rate of chemical flux from the air to the skin in Zone 2 resulting from product use in Zone 1 on the day of use.

Acute Average Gas Phase Concentration for Zone 1; $C_{g,z1a}$ (µg/cm³) One-day average concentration in Zone 1.

Acute Average Gas Phase Concentration for Zone 2; $C_{g,z2a}$ (µg/cm³) One-day average concentration in Zone 2.

Acute Dose Rate; ADR (mg/kg-day) 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 (µg/m³) 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 (m³/min) This input is the air exchange rate between near- and far-field areas in Zone 1 and governs the concentration of the chemical in the air of the far-field portion of the use environment.

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

Amount Retained on Skin; AR (g/cm²-event) The amount of product remaining on skin after use in the units of grams of product per square centimeter of skin area. This value is a function of film thickness (m) * density (g/cm³).

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} (m²) The surface area of interior surfaces such as furnishings and building materials that are potential sinks for airborne SVOCs.

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

Articles 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.

Average Chronic Gas Phase Concentration for Zone 1; $C_{g,z2c}$ (µg/cm³) The airborne concentration of the chemical in Zone 1 resulting from product use in Zone 1 averaged over one year. This could include multiple uses of the same product.

Average Chronic Gas Phase Concentration for Zone 2; $C_{g,z2c}$ (µg/cm³) The airborne concentration of the chemical in Zone 2 resulting from product use in Zone 1 averaged over one year. This could include multiple uses of the same product.

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.

Background ADR (mg/kg/d) Acute Dose Rate resulting from exposure to background concentration in air and/or dust.

Background Air Concentration (mg/m³) User specified concentration of chemical of interest within the air.

Background Chronic Dose (mg/kg-day) Chronic Dose resulting from exposure to background concentration in air and/or dust.

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

Building Volume (m³) The total volume of all rooms in the home or other building where the product or article is used. Building volume is use to estimate air concentrations of the chemical in Zone 2 (i.e., rooms where the product or article is not in use) [(U.S. EPA, 2011), Table 19-6].

Bystander A receptor who is a non-product user that is incidentally exposed to the product or article.

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; $\frac{\partial C}{\partial t}$ (µg/m³/hr) The change in the chemical concentration in air over time within a zone.

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

Chronic Dermal Flux in Zone 1; $DerFlux_{z1,c}$ (µg/cm²-hr) The rate of chemical flux from the air to the skin in Zone 1 resulting from product use in Zone 1 averaged over the course of one year.

Chronic Dermal Flux in Zone 2; $DerFlux_{z2,c}$ (µg/cm²-hr) The rate of chemical flux from the air to the skin in Zone 2 resulting from product use in Zone 1 averaged over the course of one year.

Chronic Dose; (mg/day) The receptor specific chronic dose, which is calculated by multiplying the receptor Chronic Average Daily Dose (CADD) by the receptor body weight.

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 (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 (mg/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, (cm^2) The area of an article that comes into contact with mouth.

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

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

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

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

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

Deposition Rate, RP; $kdep_{RP}$ (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 um (1-5 and 5-10) were averaged and rounded to the nearest tenth [(U.S. EPA, 2011); Table 19-33].

Dermal Absorption Dermal modeling option (P_DER2a) where dermal exposure is modeled using a fraction absorbed method.

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

Dermal Permeability Dermal modeling option (P_DERM1b) where dermal exposure is modeled using a permeability method.

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_m(min/hr) The amount of time that an article is mouthed.

Duration of Use, acute; D_{ac}(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. The minimum use duration for CEM is 0.5 minutes.

Duration of Use, chronic; D_{cr} (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.

Duration of article contact; D_{art} (min/day) The amount of time the user is in direct contact with the article throughout the day.

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.

Dust Ingestion Rate (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).

Emission Rate; ER (mg/hr) 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, 1996](#)):

- 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 μm) ([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](#)).

Incidental Soil Ingestion Rate (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 (m³/hr) The age-group-specific air inhalation rate. CEM uses separate inhalation rates for the periods during and after product use. Default values by age group are from EPA's Exposure Factors Handbook ([U.S. EPA, 2011](#)).

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

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

Initial Concentration of SVOC in Article (mg/cm^3) The SVOC additive concentration in a consumer article.

Interzonal Air Flow Rate (m^3/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.

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^2/day and 2.5, respectively. The mat used in the study for dirt collection was 0.318 m^2, so multiplying gives a geometric mean estimate of 79 mg/day in each home.

The von Lindern study estimates the amount of dirt on an entryway floor mat, but additional dirt will be tracked to the rest of the home. Thatcher and Layton (1995) provide an estimate of the rate of accumulation of dirt on a mat versus the "trackable" areas in the home. Using the relative areas of the home to get the total amount of dirt tracked per week and taking the ratio, it was estimated that 13% of the tracked dirt is on the mat and 87% is in the rest of the house.

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

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 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^2
- Children: 0.6 m^2

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

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

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

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

- $Low = 2 \times adult\ median$
- $Medium = 2 \times adult\ median + 2 \times child\ median$
- $High = 2 \times Adult\ 90th + 2 \times child\ 90th$

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_{10} 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/hr (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/use) 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.

Migration Rate of Chemical from Article to Saliva; MR (mg/cm²/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.

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

Near Field Modeling option within CEM where the model account for a small personal breathing zone around the user during product use in which concentrations are higher, rather than employing a single well-mixed room.

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™.

Peak Concentration (mg/m³) The highest concentration experienced at any point during the day of use in the use environment.

Peak Dose (mg/day) This is calculated by multiplying the receptor average daily rate (ADR) by the receptor body weight.

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

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

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. This is only use for dermal exposure models.

Product User A receptor who uses a product directly.

Radius of RP; r_{AbArt} (m) Radius of abraded particles (Little et al., 2012)

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).

Receptor The population of interest, also known as the receptor population and may be described by specific age ranges or other characteristics (e.g., gender, ethnicity, geographic location). In CEM, the receptor is limited to three age ranges, adult, youth, and child.

Resuspension Rate, Dust (per hour) 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 mm (10-25 and >25) were averaged and rounded to two significant digits [(U.S. EPA, 2011); Table 19-33].

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

Scenario User defined name for specific analysis within CEM.

Skin Partitioning Coefficients (unitless) Multiple coefficients are used to describe the portioning of a chemical between air, lipids, and multiple layers of the skin. Each is employed within the dermal air-to-skin model (A_DER1).

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

Soil Density (kg/m³) Density of soil used by CEM in calculating exposure from products applied to ground.

Soil Mixing Depth; $Depth$, (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.

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

Surface Area of Article (m²) The surface area of articles containing the SVOC. CEM provides default values for many products and articles. These can be modified by the user. Note, the model user can assume that multiple articles are present within a single room. For example, 50 toys instead of 1 toy; 2 sofas instead of 1 sofa. However, 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 (m²) Surface area of the hemispherical bubble surrounding the product user. Surface area for a use area with a radius of r is 1/2*pi. 2*pi*r^2 ([Keil and Nicas, 2003](#)).

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

Surface Area to Body Weight Ratio; $\frac{SA}{BW}$ (cm²/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 (µg/m³) For materials with an SVOC additive present at greater than 15% on a per weight basis, ([Little et al., 2012](#)) recommends using the saturation vapor pressure concentration. When the additive concentration is less than 15%, ([Little et al., 2012](#)) recommends using monitoring data to back calculate this value. Because the saturation vapor pressure concentration is the highest concentration that could be present, using this value will potentially lead to over predictions of migration. CEM uses the saturation vapor pressure in the absence of any monitoring data.

SVOC in RP Concentration; $SVOC_{RP}$ (µg/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; $SVOC_{Dust}$ (µg/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} (m³/mg) The ratio of concentrations of the chemical between dust and air at equilibrium, specific to SVOCs. If this is used in the applicable models, this value will either need to be entered by the

user based on the chemical of interest or estimated by CEM based on the volume fraction of organic matter in settled dust, the octanol-air partition coefficient for the particular SVOC, and the density of airborne particles. This value can also be estimated in the PARAMS model using vapor pressure.

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

Thickness of 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.

Use Environment The room or other location where the product/article is used.

Use Environment Volume (m³) 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 use 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].

User-defined Emission Rate (mg/hr) 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 (m³/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 Far-Field (m³) 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 (m³) The near-field volume is the portion of the use environment (Zone 1) that includes the product user and where the air concentration of the chemical is governed by emissions from product use (Keil et al., 2009; Keil and Nicas, 2003).

Water Solubility; S_w (mg/mL) A physical/chemical property defined as the amount of chemical that can be dissolved in a volume of water.

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.

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