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The Human Exposure Model (HEM)

Source-to-Dose Module

Technical Manual

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DISCLAIMER

The United States Environmental Protection Agency through its Office of Research and Development funded and collaborated in the research and development of this software. This model and its default data are currently under development; this material has been distributed for evaluation purposes only. The model has not been cleared by the United States Environmental Protection Agency for general distribution. While example input data have been provided as an example, it is up to the user to verify appropriate input data are being used for a given application. This manual is draft documentation and has not been cleared for publication.

1. Introduction

1.1 Overview

The Source-to-Dose (S2D) module is the third in a sequence of three modules which comprise the Human Exposure Model (HEM). S2D is a module for estimating aggregate exposures longitudinally. S2D employs the basic exposure scenario algorithm functions built into SHEDS-HT (Isaacs, Glen et al. 2014) to account for different exposure pathways and routes, and expands upon them to model households and primary individuals on an hourly event time step over the course of one year, while retaining daily results.

1.2 Purpose of this Technical Manual

This Technical Manual is intended to describe the logic and scientific rationale used to develop S2D. This guide will delineate the order of functions, and describe the interaction between individual functions.

1.3 Organization of this Technical Manual

The S2D Technical Manual is organized into four main sections:

1. Overview of S2D. The general structure and code design considerations are described in Sections 2-3.

2. Preparatory steps. Steps needed prior to household-level modeling can be grouped as general pre-processing steps that are performed once for all households, and steps that must be performed for each household. All preparatory steps are described in Sections 4-5.

3. Household-level modeling. For each household, route-specific exposure metrics, as well as total chemical released, and amount of chemical released to the outdoor environment are calculated. These calculations are described in Sections 6-10.

4. Overall summary. Once all households have been evaluated, overall summaries are produced that provide exposure metrics on a daily and annual basis. These summaries are described in Section 11.

2. Overview of Source-to-Dose

A detailed description of file structure, system requirements, and instructions on how to run the Source-to-Dose module can be found in the HEM User Guide.

For reference, the Source-to-Dose- module code, along with default input files, are available at: https://github.com/HumanExposure/source2dose. The 'NEW_composition_for_S2D.csv' input file is available for download at ftp://newftp.epa.gov/exposure/HEM due to it's size.

2.1 General structure of the Source-to-Dose module

The S2D module uses the R programming language to produce summaries of population-based estimates of residential exposure including contributions from individual exposure sources. The population of interest and their associated housing are specified separately in the Residential and

Population Generator (RPGen) module. Inputs for the S2D module include longitudinal patterns of consumer product use by individuals within the specified population (from the Product Use Scheduler module), chemical information for consumer products (either using the default input file or provided by the user), physical-chemical property information (from a chemical properties input file), and run settings (from the Control Module of HEM). This information is used to estimate the total chemical released; the average chemical-specific daily ingestion, inhalation, and dermal exposures; and the amount of chemical that is released to the outdoor environment and/or waste. Each exposure metric is calculated longitudinally for one year (modeled as 364 days consisting of four seasons, each of 13 weeks duration).

The general structure of the S2D module is presented in Figure 1. Following the loading of the required input datasets and pre-processing steps, the S2D module loops through all the households for the specified population. For each household, the module loops through the activity diaries of all the individuals in that specific household, and calls the Product Use function once for each product. The remaining functions are each called only once per household. In general, the output from each function is one or more R objects, containing hourly data for one household for the simulated year. These serve as inputs to other S2D functions and are deleted after use. Separate .csv files are not produced for each function within the S2D module.

The summary output, with daily and annual metrics, is reported as .csv files upon completion of the S2D module. The functions depicted in Figure 1 are briefly described in Table 1. Functions are described in more detail in Sections 6-11.

Table 1. Description of Functions within the S2D module.

Function name	Description
Product Use function: eval.use.data()	This function examines the activity diaries of all individuals in any specific household, and is run once for each unique product used by that person. Each product has an assigned product type, which determines the *a priori* release fractions for initial use phase releases, and transfers at the end of the direct use phase. Transfers during product use will depend on chemical properties. The output of the function consists of chemical mass releases to a set of compartments. See Figure 2 for a conceptual diagram representing the processing of a single product by this function.
Fugacity function: fug.concs.an()	This function uses air and surface chemical mass releases from the Product Use function, house size and house volume information from the Residential and Population Generator (RPGen) module, and inputs from databases on general house properties and chemical properties to output an hourly time series of air and surface mass of chemicals for each house. This function also determines releases into the ambient air and solid waste (from the removal of contaminated dust) from the house on a daily basis.
Direct Exposure function: eval.direct()	This function evaluates exposure during product use to the person directly using the product. It uses output from the Product Use function, including data on chemical masses in the air, residential surfaces, and skin, during and at the end of direct use phase. It also uses chemical properties and product use duration to calculate the ingestion, inhalation, and dermal exposures of the primary individual to all the chemicals of interest. There are two components to each direct exposure: during-product-use and after-product-use. In general, after-product-use exposure is due to chemical continuing to reside on the skin after product use ends. This can lead to dermal absorption, evaporation followed by inhalation, and/or ingestion via hand-to-mouth transfer.
Indirect Exposure function: eval.indirect()	This function uses air and surface chemical concentrations of chemicals as determined by the fugacity model, chemical properties and time spent in the house (from the diaries output by the Product Use Scheduler module) to calculate the ingestion, inhalation, and dermal exposures of the primary individual to all the chemicals of interest due to indirect sources.
Environmental Impact function: eval.env.impact()	This function estimates the total chemical masses contributed to the environment based on the activities that occur in the household through indoor and outdoor disposal methods. Four compartments are calculated: drain, waste, outdoor air, and outdoor surfaces.

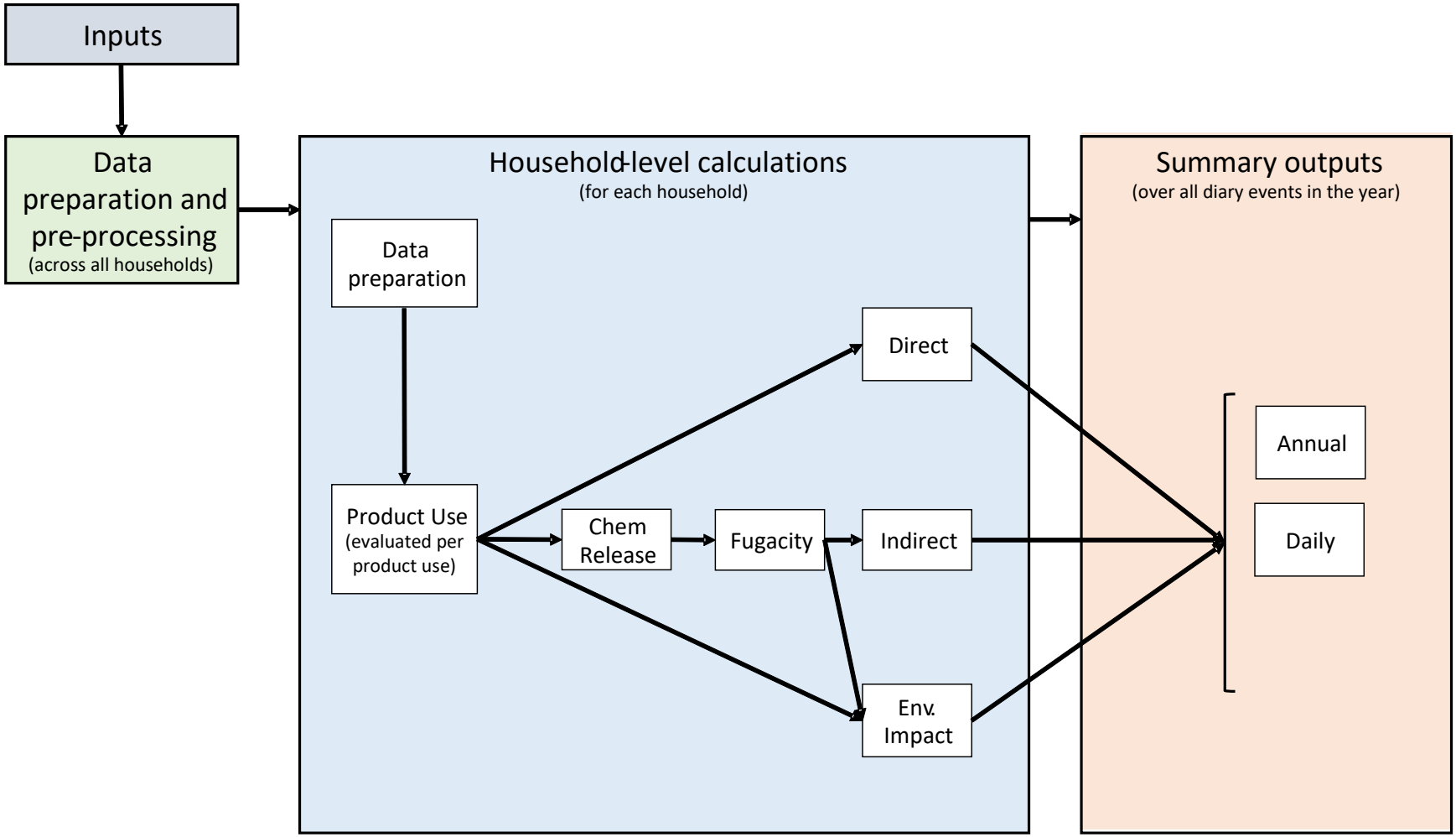

Figure 1. Flowchart of the Source to Dose (S2D) module.

2.2 Inputs

The input files required to run the S2D module are the outputs from the Product Use Scheduler and the Residential and Population Generator (RPGen) modules, and the user-provided input files on product, chemical, and housing properties.

2.2.1 Inputs from other modules

The S2D module processes outputs of various HEM modules as inputs for calculating the exposures to the primary individual in each household. These include:

1. The Product Use Scheduler module, which provides the activity diaries for every individual in the modeled households. These diaries will contain information for each day on activities over time, the product use category (PUC), product handling time, activity time, and exposure duration, as well as the product mass used, provided in files named Household_n.csv.

2. RPGen, which provides a list of household-specific properties. This includes the house location, the house size, the household income, and the household composition (the number of people in a household, adults and children, and their demographics) in a file named pophouse.csv.

2.2.2 Additional input files

Additional input files required for S2D are not dependent on other modules of HEM. Default input files, listed below alphabetically, are provided with the S2D module. If these input files are considered applicable for the desired application, then customized files must be provided by the user. A data dictionary for each input file can be found in Appendix A.

basal_vent.csv: This file contains information for estimating basal ventilation rate for household members based on age and sex.

chemical_properties_new.csv: This file contains a list of chemical properties relevant to calculating fugacity and human exposure.

Compartment_fractions.csv: This file contains the fraction of chemical that partitions into each of the 11 compartments shown in Figure 2. Product categories are sorted into one of 30 different groups dependent on how the chemicals in the product partition after use.

fugacity.csv: This file contains chemical-independent variables used to evaluate the fugacity equations.

NEW_composition_for_S2D.csv: This file contains different formulations of PUCs as well as the weight fractions of chemicals present in those formulations.

NEW_PUC_MET.csv: This file contains the associated CHAD activity code and the mean value of METS associated with product use, as calculated by APEX.

NEW_PUC_product_codes.csv: This file contains the three-letter PUC category code for each PUC, along with a product description.

NEW_PUC_skin_wipe_rinse.csv: This file describes the fractional partitioning of PUCs on the hands and/or body and how they are affected by rinsing or wiping actions.

NEW_skinsurfaceareas.csv: This file identifies which body areas are exposed to a PUC during use, per PUC. The fraction of the PUC that is associated with dermal contact on the body area specified is provided for both adults and children, as well as a simple explanation of the variability expected in the amount of dermal exposure the body area will experience.

S2D_control_file.txt: A control file for running S2D. Users will interact primarily with this file.

2.3 Outputs

Two types of output are produced for each household: daily statistics and annual statistics.

2.3.1 Daily statistics

For each chemical modeled, S2D produces a daily time series of a set of exposure variables (including the average daily ingestion, inhalation, and dermal exposures; maximum instantaneous air concentrations; and maximum instantaneous daily dermal loading of the chemicals of interest) for the primary individual, as well as daily "environmental impact" totals for solid waste, the sewer system, ambient air, and storm drains, summed over the contributions of all household members. Each household has an individual output file with a total of 23 output variables, listed in Table 2, calculated on a daily basis for each chemical. For households with exposure to more than one chemical, each chemical is listed on a separated row, and identified by its DSSTox identifier value.

Table 2. S2D Daily Time Series Output Variables

Variable name	Description of Output Variable
household	Household number from ABM output
daynum	The number of the day in a year
DTXSID	DSSTox Chemical ID
dir.derm.exp	Total mass (mg) of chemical deposited on skin from direct product use over the day
dir.derm.max	Maximum loading (mass) of chemical (mg/cm^2) present on either hands or body at any time during the day (direct use)
dir.derm.abs	Mass of chemical (mg) absorbed through skin (direct use)
dir.inhal.exp	Average air concentration of chemical (mg/m^3) for primary person associated with direct use of products
dir.inhal.max	Maximum air concentration of chemical (mg/m^3) associated with direct use of products
dir.inhal.mass	Mass of chemical (mg) inhaled over the course of the day (direct use)
dir.inhal.abs	Total mass of chemical (mg) absorbed through the lungs over the course of the day (direct use)
dir.ingest.exp	Total mass of chemical (mg) absorbed ingested from hand-to-mouth transfer as well as transferred to the gut compartment during initial use phase of products (direct)
dir.ingest.abs	Mass (mg) of chemical absorbed through the gut (direct use)
Release	Mass (mg) of chemical released by product use (by primary person only)
ind.derm.exp	Total mass (mg) of chemical deposited on skin from indirect exposure (i.e., contact with contaminated surfaces)
ind.derm.max	Maximum loading (mass) of chemical (mg/cm^2) present on either hands or body at any time during the day (from indirect exposure)
ind.derm.abs	Mass of chemical (mg) absorbed through skin (indirect exposure)
ind.inhal.exp	Average hourly air concentration of chemical (mg/m^3) for primary person (indirect exposure)
ind.inhal.max	Maximum hourly air concentration (mg/m^3) (indirect exposure)
ind.inhal.mass	Mass of chemical (mg) inhaled over the course of the day (indirect exposure)
ind.inhal.abs	Total mass of chemical (mg) absorbed through the lungs over the course of the day (indirect exposure)
ind.ingest.exp	Mass of chemical (mg) ingested from hand-to-mouth transfer (indirect)
ind.ingest.abs	Mass of chemical (mg) absorbed through the gut (indirect)

Variable name	Description of Output Variable
out.sur	Mass of chemical (mg) released to outdoor surfaces (outdoor product use)
out.air	Mass of chemical (mg) released to outdoor air (outdoor use and house losses)
drain	Mass of chemical (mg) going into the drain system (includes chemical in the hair and nail compartments)
waste	Mass of chemical (mg) disposed in trash

2.3.2 Annual statistics

In addition to daily statistics, S2D also outputs annual statistics for the primary individual. The list of output variables is the same as for the daily summary statistics, shown in Table 2 above, except that the annual statistics does not have a daynum variable, since it is an annual summary. One file is generated for each household, with each chemical on a separate row. For model runs where more than one household is exposed to the chemicals of interest, an annual statistics file is created for all households. At the end of processing each household, the final exposure data for that household is recorded in a .csv file that covers all households. If HEM is run on a cloud server which allocates a different set of households to each of several processors, the output from each processor may be saved in a separate file, and these files may be joined together when the S2D calculations are completed.

2.4 Code design considerations

A full HEM run is likely to consist of several chemicals and thousands of households. The various chemicals to which people are exposed in the S2D module are not independent of each other, since frequently more than one chemical exists in a given product. Thus, parameters such as product mass, frequency, and use duration are shared across chemicals. However, each household is independent and therefore, different households can be modeled on different processors. To reduce processing time, the S2D code was developed in R to allow for parallel processing. For example, if a sample of 1000 households was created, it would be possible to have 10 computers each run 100 different households through the S2D calculations. The option of parallelization is available by turning this feature on or off in the control file. Outputs from different processors are then aggregated together.

2.5 Uncertainty and variability

As the user considers uncertainty and variability of model outputs, a few points to consider. The current inputs for the S2D module should be interpreted as representing variability among individuals (e.g., use parameters) or among products (e.g., weight fractions), and do not per se reflect uncertainty. Many of the model inputs for use assume a fixed coefficient of variation to account for variation among individuals. As is typical with consumer product models, the exposure is most sensitive (linearly related) to mass and frequency of application. Similarly, exposure is linearly weighted to weight fraction of the chemical in the product. Significant parameter uncertainty may be imparted by lack of data in these areas (e.g., categories for which these data are assumed) or by bias or lack of representativeness in the available information. For example, the set of products for which weight fraction data are available may not (is likely not) representative of products in commerce. Therefore, we are focusing our current efforts

to identify additional data in the product use and composition realms (especially for poorly-studied product categories) allowing us to improve our estimation of variability among individuals and products, while at the same time provide us new information that could allow us to develop compatible combinations of central tendencies and variance characteristics that could be implemented in a 2-Dimensional (2D) Monte Carlo evaluation of the impact of parameter variability and uncertainty. Other sources of uncertainty arise from model (algorithm) selection, which is harder to quantify and will be a focus in the future. Planned model evaluation exercises, including comparison of modeled data from various modules to reported or measured information, could inform uncertainty analyses (e.g., by providing a basis for reasonable uncertainty bounds on intermediate variable estimates entering the S2D module. Batch mode capability and the text-based input format of HEM currently would allow for the external implementation of a 2D probabilistic assessment at any time.

3. Random number sampling and reproducibility

3.1 Overview

HEM is a stochastic exposure model in which many variables are randomly sampled from distributions. The S2D module currently considers over 300 unique product categories (PUCs). The default composition file provided with the module includes multiple representative products per product category. Representative products and their formulations are taken from data contained in the CPDat database (Dionisio, Phillips et al. 2018). See Appendix A for details on the composition input file.

When the product use diaries identify a PUC as being used by a given household, a representative product and a formulation for that product are randomly selected from the data provided in the input file. A single formulation may contain for example, 5-10 chemicals, however there may be >100 chemicals represented within a single PUC across all representative products. With model runs that consist of multiple chemicals and thousands of households, a single run of the S2D module may take up to one hour per household if the number of chemicals is large. A useful feature is the ability to split runs into parts by focusing on a small number of chemicals in one model run. Another batch of chemicals can then be run using the same population and household product use diaries for the same PUC.

To allow the user to split the model run into several parts, while still retaining the same selection of representative product and chosen formulation (from the 100 formulations for that representative product), the S2D module allows the user to have control over certain aspects of the random number generation used to select representative product and formulation. Random number functions return one or more random values (called a “stream”) from a “seed” value. Generally, the seed is an integer ranging from 1 up to some specific limit (dependent on the language and specific generator), while the random values are real numbers uniformly distributed between zero and one.

To achieve the goal of fully reproducible runs, separate seeds, and hence separate streams of random numbers were created for each modeling variable. In practice, this means that each household, each product (or PUC), and each chemical, receives its own seed, based on the overall seed that the user assigns for the run. Then more runs can be performed with selected changes, without impacting the

other parts of the run. For example, the chemical list may be expanded (or reduced), and the results for the chemicals common to both runs should be the same.

3.2 Creation of random variables: get.ran.vars()

This function makes a list of random variables in each of the three categories which require seeds. The categories are household variables (Table 3), product variables (Table 4), and chemical variables (Table 5). The household variables are any which require just one sample per household (detailed in Table 3, below).

Table 3. Household variables.

Variable	Description
aer.out	Air exchange rate with outdoors
height	Average ceiling height
lg.carb.f	Organic carbon fraction in large (dust) particles
lg.clean.air	Cleaning rate for large airborne particles
lg.clean.sur	Cleaning rate for large particles on surfaces (dust removal)
lg.depos	Deposition rate on floor for large airborne particles
lg.load.air	Loading in air for large airborne particles
lg.load.sur	Loading on floor for large particles
lg.resus	Resuspension rate (floor-to-air) for large particles
sm.carb.f	Organic carbon fraction in small particles
sm.clean.air	Cleaning rate for small airborne particles
sm.clean.sur	Cleaning rate for small particles on surfaces
sm.depos	Deposition rate on floor for small airborne particles
sm.load.air	Loading in air for small airborne particles
sm.load.sur	Loading on floor for small particles
sm.resus	Resuspension rate (floor-to-air) for small particles
temp	Indoor temperature
thick.bou	Boundary layer thickness over floor
thick.sur	Effective thickness of floor (for chemical penetration)
basal.vent	Basal ventilation rate for primary person in household
hand.wash	Hand washing frequency for primary person
hand.mouth	Hand mouthing frequency for primary person

For each product in the model run there are three product related variables, detailed in Table 4, below.

Table 4. Product variables.

Variable	Description
prod.id	Chosen representative product in the PUC
form.id	The specific chemical formulation
skin.frac	The fraction of the skin area to which the product is applied

Get.ran.vars() distinguishes the products by assigning a numerical suffix. Thus, the third product in the list for this run has variable names “prod.id3”, “form.id3”, and “skin.frac3”.

For each chemical in the model run there are six chemical related variables, detailed in Table 5, below.

Table 5. Chemical variables.

Variable	Description
vapor	Chemical vapor pressure
solub	Solubility
kow	Octanol-water partition coefficient
decay.air	Chemical decay rate in air
decay.sur	Chemical decay rate on surfaces
diffus.air	Diffusivity in air

As for products, each is assigned a numerical suffix to distinguish between chemicals. For example, in a run with 3 PUCs and 5 chemicals, get.ran.vars() returns a list of 61 variable names (22 household variables (each detailed in Table 3), 3 product related variables (each detailed in Table 4) for each of the three PUCs of interest, and 6 chemical related variables (each detailed in Table 5) for each of the 5 chemicals of interest).

3.3 Creation of seeds: get.seeds()

As explained above, get.seeds() starts with the initial run seed, and produces two 32-bit seeds for each variable name returned from the get.ran.vars() function. In the above example (3 PUCs and 5 chemicals), this is a list of 61x2 = 122 seeds, each of 32 bit length. Calculated seeds will be out of range if the number of PUCs and/or number of chemicals exceeds one million.

3.4 Creation of random numbers: get.randoms()

The function creates a matrix, with one column for each variable returned by get.ran.vars(), and one row for each household in the run. All the numbers are between zero and one. Each column represents one stream of random numbers. The numbers within each column should be independent by the nature of the random number generator. The numbers across columns should be independent due to the steps taken to produce unrelated seeds for each column.

3.5 Random values from distributions: distrib()

The distrib() function was originally written for the SHEDS-HT model (Isaacs, Glen et al. 2014). It has two purposes: to produce random values from a list of distributions (including the empirical or discrete), or to return specific quantiles from any of the distributions, whether truncated or not. This has several advantages over using the generic random number functions in R, such as rnorm() and qnorm(). First, those functions support just one type of distribution, so the code would have to be changed if the user changed the type (say, from normal to lognormal). Second, those functions generally do not support truncated forms.

Distrib() has a total of 12 arguments, but some are optional. When calling distrib(), the arguments (detailed in Table 6), may be listed in order without keywords, provided that any skipped are indicated by consecutive commas. As a general rule, the arguments should be used with their keywords for clarity.

Table 6. Arguments for the distrib() fuction.

Keyword	Options	
Shape	Usually omitted. It is a text string (with quote marks) indicating the form of the distribution. Only the first four characters are retained, and case is not important. The recognized choices and the number of required parameters are:	
	Bern:	Bernoulli distribution, one parameter. If missing, assumed = 0.5 Returns 1 with chance= par1, else returns 0.
	Bino:	Same as Bern.
	Beta:	Beta distribution with up to 4 parameters. Par1 and Par2 are the shape parameters. Par3 is the lower bound and Par4 is the upper bound. Often, Beta is called with just Par1 and Par2, when the range is the default 0 to 1.
	Disc:	Returns one of a discrete set of values. The list of values is supplied as a vector v, and the list of probabilities for each is supplied as the vector p. V may be either numeric of character.
	Empi:	Empirical distribution. Each value in the vector v is equally likely to be chosen.
	Expo:	Exponential distribution. Par1 is the decay rate, par2 is the shift (which is zero if omitted), and par3 is the upper truncation limit.
	Gamm:	Gamma distribution. Par1 is the shape, par2 is the scale, and par3 (if present) is the upper truncation limit.
	Logn:	Lognormal distribution. Par1 is the geometric mean GM, and par2 is the geometric standard deviation GSD, which must exceed 1. An optional par3 (usually zero) shifts the distribution.
	Norm:	Normal distribution. Par1 is the mean, and par2 is the standard deviation.
	Poin:	Point value, which always equals par1.
	Prob:	Essentially this is a discrete distribution without a preset list of values to return.
		The return value is numeric, and reflects the position of the selected item.

Keyword	Options	
	Tria:	Triangle distribution. Par1 is the minimum, the lesser of par2 and par3 is the peak, and the greater of par2 and par3 is the maximum.
	Unif:	Uniform distribution between par1 and par2.
	Weib:	Weibull distribution. Par1 is the shape parameter and par2 is the scale parameter. An optional par3 shifts the distribution.
Par1 – Par4	Numerical parameters with meanings that depend on the shape (see above).	
Lt	Lower truncation limit.	
Ut	Upper truncation limit.	
Resamp	Rule for handling generated values beyond the truncation limits. If "Y" (the default), then the distribution is essentially resampled until the value is within the limits. This means that the probabilities for all values between the limits are enhanced. If resamp="N" then values beyond the limit are moved to the appropriate limit. This may result in a probability spike at the limit, as the tail area is "piled up" there.	
N	The number of samples requested. All must use the same arguments. Distrib() does not support a list of N shapes in a single call, for example. Either N or Q is required, and determines the mode of operation. Using N, distrib() generates random samples. Using Q, distrib() transforms numbers in a deterministic manner.	
Q	A list of quantiles to be returned. Quantile are like percentiles, except they range from zero to one. Q=0.5 is the median, and q=0.99 is the 99th percentile. Q may be specified to many decimal places, limited by machine precision.	
P	A vector of probabilities, used only with the "disc" or "prob" shapes.	
V	A vector of values to be selected from, either numeric or character. Used only with the "disc" or "empi" shapes.	

3.6 Using random number control in Source-to-Dose

Random number control has been implemented within the Source-to-Dose module. The S2D code must be supplied with either one overall initial seed, or three separate seeds (for households, products, and chemicals). There is no loss of randomness by using one overall seed for all three, as each variable is assigned a unique seed, different from all other variables. The reason for allowing separate initial seeds for each set is that sometimes the user may want to keep the random variables exactly the same for one set of variables, while altering another. This is particularly useful in sensitivity analysis. Both the one initial seed and three initial seed cases are referred to collectively when the terms "initial seed" or "run seed" are used. In the three-seed case, the term "initial seed" should be interpreted as "initial seed for

variables in this class." The 22 randomly sampled household variables in S2D have seeds that depend on the overall run seed and the starting house number. For example, if one S2D run covers houses 1-100 and the second covers houses 51-100, then all the houses in the second run should match the second half of the first run. Similarly, Each PUC has a seed determined by the run seed and a unique PUC-specific number, and each chemical has its own unique number. Hence, if the same PUC or chemical appears in two S2D runs with the same run seed, then the random numbers assigned to that PUC or chemical will be the same.

The repeatability described above is convenient, but in some cases might lead to unintended consequences. For example, if one is in the habit of running the same PUC in many runs (for any reason), then note that the same product.id (representative product) and formulation.id (formulation) will be assigned every time to the corresponding household. If one intends to use multiple runs to build up a larger random sample (because, say, there are hundreds of representative products available for that PUC), then one should vary the run seed between runs so that a different representative product is picked in each run.

4. General pre-processing steps

Prior to modeling of household exposure, general pre-processing steps must first be performed. These steps are performed only once in the model and their outputs are applicable for all households. The 19 pre-processing steps have been grouped into four categories: PUC-specific parameters, chemical properties, household information, and calendars.

4.1 Product use category (PUC) specific parameters

The nine functions that provide product use category specific parameters are described below.

4.1.1 Input data

The following six functions read various input files:

read.compart.fracs() reads a .csv file of initial compartmental fractions by PUC.

read.puc.met() reads the input file containing the mean MET value for each PUC.

read.vent.file() reads the .csv file with basal ventilation rates in m^3/day.

read.puc.types() reads the .csv file listing the product type for each PUC.

read.removals() reads the file with rinse-off and wipe-off fractions by PUC.

read.skin.areas() reads the file with affected skin area fractions by PUC.

4.1.2 Evaluation of representative products and formulations: eval.brand.list()

This function evaluates the representative products (by product.id) and formulations to be retained for the user-defined run based on the user-defined chemicals and PUCs of interest. The function generates a list of representative products for each PUC being studied that contain the chemicals being studied.

The representative products for each PUC are listed on the composition input file, identified by numeric codes. A PUC may have anywhere from one to several hundred representative products. By default, or under comp.method=1 on the control file, all representative products present in the composition file for a given PUC are equally likely to be selected. A single representative product is randomly selected for each household, and all persons in that household use the same representative product if they are a user of that PUC. Independent representative product selections are made for each household.

Inputs

chem.list	all the chemicals
puc.list	all the PUCs
chem.fracs	mass fraction of the chemical in the representative product and formulation

Outputs

brand.list	list of all representative products (by product.id) for each PUC being studied, which contain the chemical(s) being studied

4.1.3 Evaluation of representative products and formulations to retain: reeval.brand.list()

This function shortens the list of representative products and formulations to be retained if the user selects the option comp.method=2 in the control file. In this case, the list of representative products (by product.id) for each PUC is shortened to include only those representative products which contain the chemical of interest for the model run. This ensures that, for comp.method=2, each individual who is a user of the PUC being modeled has a non-zero exposure to the chemical of interest.

4.1.4 Compartmental fraction releases by PUC: eval.release.fracs()

This function lists the compartmental fractional releases for each PUC. These compartments form the top row of Figure 3 in section 6.3 below. These fractions are taken to be the same for all representative products, formulations, and chemicals. The reason is that the nature and purpose of the product category determines where the product is initially released when used. The second and third levels of Figure 3 may reapportion the chemicals, based on chemical properties, product mass, affected area, use duration, and the resulting calculated flow rates.

4.1.5 Hand-to-mouth transfer: eval.hm.rate()

The hand-to-mouth transfer rate constants are calculated in this function.

Inputs

prime	demographic information on the primary individual and exposure factors such as basal ventilation rate, skin surface area, hand washing, and hand to mouth transfer rates
q	randomly sampled house, PUC, and chemical variables for the specific household

Outputs

props	information on the molecular weight, vapor pressure, solubility, octanol-water partition coefficient, air and surface decay constants, and diffusion constant for all the chemicals.

Hand-to-mouth transfer rate constants for the primary person in each household were calculated by using results from a custom version of EPA's SHEDS-Multimedia model designed to predict soil and dust ingestion rates (Ozkaynak, Xue et al. 2011). S2D assumes that adults have the same hand-to-mouth transfer rate as 16-20 year olds. The hand-to-mouth rate constants used were determined by model run results to lognormal distributions, and assuming that the fractional rate per hour is one-half of the ratio found empirically in those model runs (hand-to-mouth exposure to hand exposure). The fitted geometric mean and geometric standard deviation are presented below in Table 7. The rate constants (in units of 1/hr) are taken to be one half of the resulting values sampled from these distributions.

Table 7. Hand-to-mouth distribution parameters for the primary person in each household.

Age (years)	GM (unitless)	GSD (unitless)
0	.2	1.8
1	.23	1.7
2	.19	1.9
3-5	.15	1.9
6-10	.09	2.0
11-15	.05	2.4
16+	.02	3.1

4.2 Chemical properties

The four functions that provide chemical-specific parameters are described below.

4.2.1 Input data

The two functions that read various data input files into the S2D model are listed below:

read.chem.fracs() loads the .csv file of chemical fractions in each product.

read.chem.props() reads the .csv file of chemical properties and performs simple calculations to convert the following: log K_{ow} to K_{ow}, and half-life values for sediment and air into decay constants.

4.2.2 Evaluation of chemicals to be retained: eval.chem.list()

This function evaluates the chemicals and retains only those chemicals that are present in the PUCs.

Inputs

chem.list	all the chemicals
puc.list	all the PUCs
chem.fracs	mass fraction of the chemicals in all brands and formulations of the PUCs

Output

chem.list	list of all chemicals that are present in the PUCs

4.2.3 Evaluation of chemical properties: eval.chem.props()

The chemical properties function randomly samples chemical properties from distributions based on the "chemical_properties_HEM.csv" input file.

Inputs

fug.cvars	chemical properties of each chemical
chem.list	all the chemicals
ran.vars	a list of house, PUC, chemical related variable names that rely on random value generation in the modeling process
q	randomly sampled house, PUC and Chemical variables for the specific household

Outputs

props	each chemical is identified by its DTXSID code and includes the properties listed in Table 8

Table 8. Relevant chemical properties for each chemical.

Variable name	Units	Description of output variable
molwt	g/mol	molecular weight
vapor	Pa	vapor pressure
solub	mol/m^3	Solubility
kow	-	octanol-water partition coefficient
decay.sur	1/day	chemical decay on surfaces
decay.air	1/day	chemical decay in indoor air
diffus.air	m^2/day	chemical diffusivity in air

Several variables from the chemical properties input file are in different units or forms from the target output. Accordingly, the following conversions are performed internally in the S2D code.

Solubility is converted from milligrams per liter to moles per cubic meter as follows:

$$solub\ \left[\frac{\text{mol}}{\text{m}^3}\right] = \frac{solub\left[\frac{\text{mg}}{\text{L}}\right] * 1000\ \text{L/m3}}{molwt * 1000\ \text{mg/g}} \quad (1)$$

where:

$solub$ = solubility
$molwt$ = molecular weight [g/mol]

The octanol-water partition coefficient is derived from the log(kow) variable on the input file by converting from base 10 logarithm:

$$K_{ow} = 10^{\log(kow)} \quad (2)$$

where:

K_{ow} = octanol-water partition coefficient [-]
$\log(K_{ow})$ = base 10 logarithm of octanol-water partition coefficient [-]

The air and surface decay rates are derived from reported half-lives as shown below. The air half-life is given directly on the input file, although it does not distinguish between indoor and outdoor air. The surface half-life is taken to be the sediment half-life from the input file.

$$decay.sur\ \ OR\ \ decay.air = \frac{\log(2)}{halflife} \times 24 \quad (3)$$

where:

$decay.rate$ = chemical decay rate on surfaces or in indoor air [day^{-1}]
$halflife$ = chemical half-life [hr]
24 = conversion factor from hrs to days

The chemical diffusivity in air is calculated from other chemical properties, using the equation. An additional conversion factor is used in S2D in order to have units of m^2/day.

$$diffus.air = \frac{2.05 \times \sqrt{\frac{1}{29} + \frac{1}{molwt}}}{molwt^{0.33}} \times \frac{86{,}400}{10{,}000} \quad (4)$$

where:

$diffus.air$	=	chemical diffusivity in air [m^2/day]
$molwt$	=	molecular weight [g/mol]
$86{,}400$	=	conversion factor from days to seconds
$10{,}000$	=	conversion factor from m^2 to cm^2

4.3 Household information

The three functions that provide household information are listed below:

read.diary() loads the product-use diary for one household.

read.fug.inputs() reads the .csv file of chemical-independent fugacity variables.

read.pophouse() reads the output from the HEM RPGen module.

4.4 Calendar

Three functions that generate calendars are described in this section.

4.4.1 Make calendars

The two functions that make a day and hourly calendar are listed below:

make.day.calendar() creates a 364 day long standard calendar.

make.hour.calendar() creates a calendar of 364 days, 24 hours each day.

4.4.2 Evaluation of chemical releases: eval.chem.release()

The chemical releases function creates an hourly calendar with all the chemical releases in the household, based on the chemical use data of the individuals in the household.

Inputs

pucs	only those PUCs that are part of the house diary (for any specific house being evaluated in the loop over houses), with related information, for example, the PUC code
use.data	chemical masses, with one dimension each for the number of PUCs being used by the household, the use phase (duration over which the product is actually being used), number of compartments to which the PUC releases chemical to, and the number of chemicals in the specific brand and formulation of the PUC that has been randomly chosen for the household
use.chem	total mass of each chemical released by each PUC's use in the household
compart.list	names of the 11 compartments that are being modeled as part of the mass partition approach
diary	activity diaries of all the individuals in the household, output from the Product Use Scheduler module

nc	number of chemicals being modeled in the current model run
calendar.hours	hourly calendar for 364 days with information on the hour number, day number, season, week, hour, day of the week, and a binary tag for a weekend.

Outputs

Chemical masses in the air, surface, air and surface combined, and all the compartments together for each hour in a calendar year.

5. Data preparation for household-level calculations

The following functions are performed for each household.

5.1 Evaluation of house properties: eval.house.props()

The house properties function randomly samples house properties from distributions on the fugacity input file, except for total floor area which comes from the pophouse.csv input file which includes characteristics of the residence.

Inputs

fug.hvars	distributions produced by the read.fug.inputs() function
person.data	demographic data produced by the read.pophouse() function
q.randoms	random quantiles produced by get.randoms() function

Outputs

house.props	values of the twenty house property variables (see Table 9 below).

Table 9. House variables evaluated.

Variable name	Units	Description of output variable
aer.out	1/day	indoor-outdoor air exchange rate
area.sur	m^2	total floor area
Height	m	average ceiling height
lg.carb.f	-	carbon fraction in large particles
lg.clean.air	1/day	large particle removal rate for air
lg.clean.sur	1/day	large particle removal rate for surfaces
lg.depos	m/day	large particle deposition rate (air to surface)
lg.load.air	$\mu g/m^3$	large particle loading in air
lg.load.sur	$\mu g/m^2$	large particle loading on surfaces
lg.resus	1/day	large particle resuspension rate (surfaces to air)
sm.carb.f	-	carbon fraction in small particles
sm.clean.air	1/day	small particle removal rate for air
sm.clean.sur	1/day	small particle removal rate for surfaces

Variable name	Units	Description of output variable
sm.depos	m/day	small particle deposition rate (air to surface)
sm.load.air	μg/m^3	small particle loading in air
sm.load.sur	μg/m^2	small particle loading on surfaces
sm.resus	1/day	small particle resuspension rate (surfaces to air)
Temp	K	indoor temperature in degrees Kelvin
thick.bou	m	thickness of boundary layer over surfaces
thick.sur	m	effective thickness of surface compartments

Three variables require a unit conversion from the pophouse.csv input file (generated from RPGen) to the S2D outputs and are listed below:

$$area.sur = \frac{unitsf}{10.7639} \tag{5}$$

$$lg.load.sur\left[\frac{\mu g}{m^2}\right] = lg.load.sur\left[\frac{\mu g}{cm^2}\right] \times 10{,}000 \tag{6}$$

$$sm.load.sur\left[\frac{\mu g}{m^2}\right] = sm.load.sur\left[\frac{\mu g}{cm^2}\right] \times 10{,}000 \tag{7}$$

where:

$area.sur$ = floor area [m^2]
$unitsf$ = floor area [ft^2]
$lg.load.sur$ = large particle surface loadings
$sm.load.sur$ = small particle surface loadings
$10{,}000$ = conversion factor from mg/cm^2 to mg/m^2

The average ceiling height is sampled from a standard distribution that includes both regular and high ceilings. It is planned that the high ceiling indicator on the RPGen output will be used to separate this into two distributions (for regular and high ceilings).

The remaining house properties are sampled in the same units given on the input file.

5.2 Evaluation of chemical flow rates in the house: eval.flows()

The chemical flows function determines the flow rate constant for four flows and are part of the calculations in the fugacity function.

Inputs

hp — values for the house properties variables. One record only for the house being considered (isolated from the house.props dataframe).

Chem.props — information on the molecular weight, vapor pressure, solubility, octanol-water partition coefficient, air and surface decay constants, and diffusion constant for all the chemicals.

Outputs

Flow rate constants for surface to air transfer, air to surface transfer, total loss rate for air, and total loss rate for surfaces (detailed in Table 10).

Table 10. Chemical flow rate constants.

Variable Name	Units	Description of Output variable
a	1/day	total loss rate for air
b	1/day	surface to air transfer
c	1/day	air to surface transfer
d	1/day	total loss rate for surfaces

5.2.1 Overview of flows

The flow rates are specific to each house and determine how quickly chemical moves from one compartment to another, where compartment is defined as either air or surface. The air and surface compartments are connected to each other, and are also connected to the outdoors. In S2D, the air and surface compartments collectively represent the interior of a house. Each compartment consists of three “phases”, which are bulk, small particles, and large particles. For the air compartment, the bulk phase is chemical in the vapor phase, while the small and large particles represent airborne dust containing particle-bound chemical. For the surface compartment, the particles form a surface layer of "dust" which is not bound to the surface and therefore capable of moving into the air.

Chemical moves between the indoor and outdoor air compartments by air exchange. In this model, air exchange always has equal volume in each direction. Outdoor air is assumed to contain no chemicals of interest. However, the outdoor air is assumed to contain the same amount of particles as the indoor air. This is important because the model insists on particle balance, that is, the mass of particles in each compartment is constant in time. Chemical moves from air to surfaces by particle deposition, or from surfaces to air by resuspension. Chemical may also transfer directly (by evaporation or condensation), without being bound to dust. Each compartment is assumed to be in internal equilibrium, meaning that its phases are always at the same fugacity as each other.

The flow rates are normalized to unit chemical mass, and therefore depend only on the house properties and chemical properties (see Sections 5.1 and 4.2.3). In S2D, it is assumed that all house and chemical properties are constant in time, which means that the flow rate constants are also constant in time. Note that the actual chemical flows change with time because they are given by the product of the (constant) flow rates and the (varying) chemical masses in the relevant compartments. To calculate the

four flow rate variables [a, b, c, d] for air to surface, surface to air, total loss from air, and total loss from surfaces, S2D models chemical flows as shown in Figure 2.

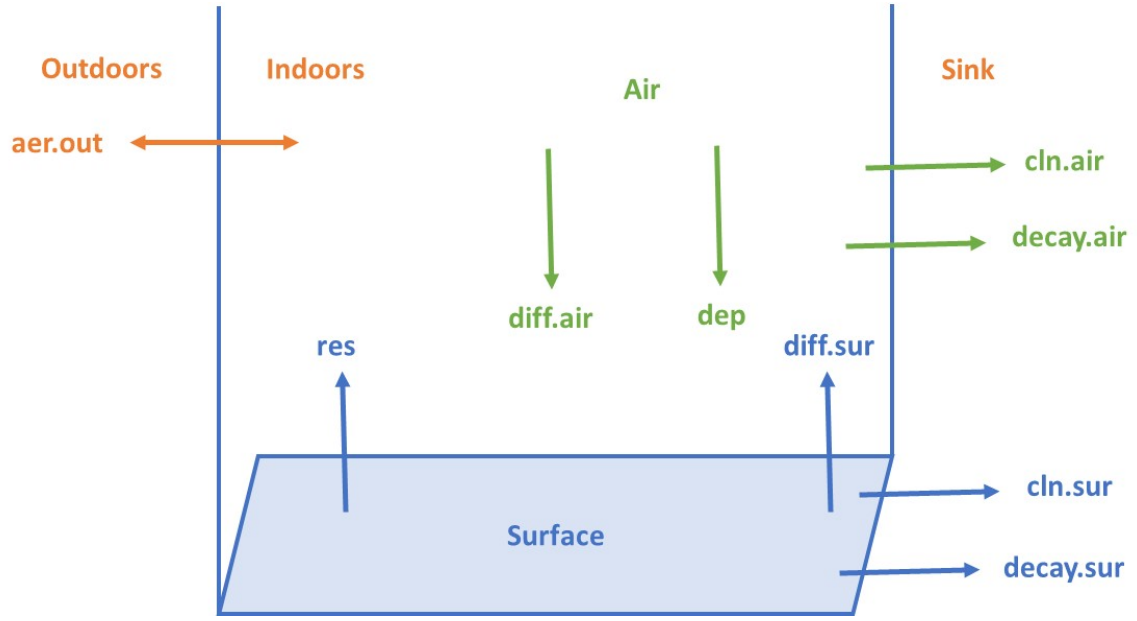

Figure 2. Flow compartments.

The flow rate constant for each of the four "flow compartments" is calculated as the summation of the individual flow rate constants as follows:

$$a = aer.out + decay.air + cln.air + dep + diff.air \quad (8)$$

$$b = res + diff.sur \quad (9)$$

$$c = dep + diff.air \quad (10)$$

$$d = decay.sur + cln.sur + res + diff.sur \quad (11)$$

where:

a	=	total loss rate for air [1/day]
b	=	surface to air transfer [1/day]
c	=	air to surface transfer [1/day]
d	=	total loss rate for surfaces [1/day]
$aer.out$	=	indoor outdoor exchange rate [1/day]
$decay.air$	=	chemical decay in air [1/day]
$decay.sur$	=	chemical decay on surface [1/day]
$cln.air$	=	overall cleaning rate in air [1/day]
$cln.sur$	=	overall cleaning rate on surfaces [1/day]
dep	=	total deposition on floor [1/day]
res	=	total resuspension [1/day]
$diff.air$	=	diffusion from air to floor [1/day]

$diffsur$ = diffusion from floor to air [1/day]

Of the nine variables used in the equations 8-11, the indoor outdoor exchange rate is obtained from the house properties function (see Section 5.1), while the chemical decay rates in air and on surfaces are obtained from the chemical properties function (see Section 4.2.3). The remaining six variables are calculated within the chemical flows function and described in Section 5.2. To determine these variables, S2D calculates and saves many intermediate variables which is described below, along with the concepts needed for the calculations of the intermediate variables.

5.2.2 General relationship between chemical mass and fugacity

In S2D, each compartment (air or surface) consists of three phases: bulk, small particles, and large particles. Chemical in the bulk phase is in vapor form for air, or embedded in the flooring material for surfaces. Chemical may also be bound to either small or large particles (dust), either airborne or on surfaces. A key assumption in this model is that all three phases in a given compartment are always at the same fugacity as each other, although this common compartmental fugacity may change over time. However, different compartments will generally have different fugacities.

$$F_{bulk} = F_{sm} = F_{lg} = F_{comp} \quad (12)$$

where:

F_j = fugacity in phase *j* [Pa]

j = phase corresponding to bulk, small particles (sm), large particles (lg), and overall air or surface compartment (comp)

The fugacity depends on the material properties, the amount of material present in that phase (represented by its volume), and the chemical mass in that phase. The basic relationship is:

$$M_c = F \times Z \times V \quad (13)$$

where:

M_c = mass of chemical [mg]

F = fugacity [Pa]

Z = fugacity capacity [[mg/m^3/Pa]

V = volume [m^3]

The same equation may be used if both M_c and Z use grams or moles, rather than micrograms. The S2D code uses micrograms to avoid outputs that could otherwise be very small, requiring exponential notation.

All properties of a compartment apart from the chemical mass and fugacity are assumed to be constant in time. Hence, the Z and V terms for all phases and compartments are constant in time, but M_c and F are not constant in time. For each compartment, since Z and V are constant in time, M_c and F exhibit the same functional time behavior as they always have a fixed ratio.

$$Z \times V = \frac{M_c}{F} = constant \quad (14)$$

5.2.3 Fugacity capacity

The following equations in this section originate from Bennett and Canales (Bennett and Canales 2004).

The fugacity capacity of pure air (without particles) is given by:

$$z.air = \frac{1}{R \times temp} \quad (15)$$

where:

$z.air$	=	fugacity capacity of air; molar density in pure air [mol/Pa/m^3]
R	=	ideal gas constant, 8.314 [Pa-m^3/mol-K]
$temp$	=	temperature [K]

For surfaces, the fugacity capacity of surfaces (molar density on surfaces) is a blend of two regressions for hard flooring and for carpet (Bennett and Canales 2004). The original equations were for the dimensionless partitioning coefficient between floor and air, so they have been converted below to fugacity capacities by multiplying by $z.air$:

$$z.sur = \frac{z.air \times 82{,}500}{vapor^{0.65}} \quad (16)$$

where:

$z.sur$	=	fugacity capacity of surface; molar density on surface [mol/Pa/m^3]
$vapor$	=	vapor pressure [Pa]

5.2.4 Mass-to-fugacity ratios

For mass to fugacity ratios, the "zv" variables in the below equations represent the product of Z and V in equation 14. One such variable exists for each compartment and represents the ratio of chemical mass to fugacity. The mass to fugacity ratio of air is composed of three individual mass to fugacity ratios corresponding to that of: (i) the pure compartment, (ii) small particles in air, and (iii) large particles in air. The same three components are needed to calculate the mass to fugacity ratio of surfaces.

From Bennett and Canales, the mass to fugacity ratio to bulk (vapor phase) air and to surfaces is given by:

$$zvb.air = z.air \times vol.air \times ug.mol \quad (17)$$

$$zvb.sur = z.sur \times area.sur \times thick.sur \times ug.mol \quad (18)$$

where:

$zvb.air$	=	mass to fugacity ratio for pure air [mg/Pa]
$zvb.sur$	=	mass to fugacity ratio for surface [mg/Pa]
$area.sur$	=	total floor area [m^2]
$thick.sur$	=	effectiveness thickness of surface compartments [m]

The unit capacities, which correspond to the fugacity capacity per unit mass, are constant for each particle size regardless of location, and are given below. The particle-air partition coefficients used in the equations below are described in Section 5.2.5.

$$sm.cap = z.air \times sm.kp \times ug.mol \quad (19)$$

$$lg.cap = z.air \times lg.kp \times ug.mol \quad (20)$$

where:

$sm.cap$	=	unit capacity for small particles [1/Pa]
$lg.cap$	=	unit capacity for large particles [1/Pa]
$sm.kp$	=	particle-air partition coefficient for small particles [m^3/mg]
$lg.kp$	=	particle-air partition coefficient for large particles [m^3/mg]

The ratio of mass to fugacity for small and large particles in the air compartment is given by:

$$sm.zv.air = zvb.air \times sm.kp \times sm.load.air \quad (21)$$

$$lg.zv.air = zvb.air \times lg.kp \times lg.load.air \quad (22)$$

where:

$sm.zv.air$	=	mass to fugacity ratio for small particles in air [mg/Pa]
$lg.zv.air$	=	mass to fugacity ratio for large particles in air [mg/Pa]
$sm.load.air$	=	small particle loading in air [mg/m^3]
$lg.load.air$	=	large particle loading in air [mg/m^3]

The ratio of mass to fugacity for small and large particles in the surface compartment is given by:

$$sm.zv.sur = sm.cap \times sm.mass.sur \quad (23)$$

$$lg.zv.sur = lg.cap \times lg.mass.sur \quad (24)$$

where:

$sm.zv.sur$	=	mass to fugacity ratio for small particles in surface [mg/Pa]
$lg.zv.sur$	=	mass to fugacity ratio for large particles in surface [mg/Pa]
$sm.mass.sur$	=	small particle mass on surfaces [mg]
$lg.mass.sur$	=	large particle mass on surfaces [mg]

The ratio of mass to fugacity for the entire air compartment is the summation of the mass to fugacity ratio of pure air and the mass to fugacity ratios of small and large particles in air. The equation for mass to fugacity ratio for the entire surface compartment is similar.

$$zv.air = zvb.air + sm.zv.air + lg.zv.air \quad (25)$$

$$zv.sur = zvb.sur + sm.zv.sur + lg.zv.sur \quad (26)$$

where:

$zv.air$ = mass to fugacity ratio for air [mg/Pa]
$zv.sur$ = mass to fugacity ratio of surfaces [mg/Pa]

5.2.5 Partition coefficients

Air-surface. The air-surface partition coefficient was previously described in Section 5.2.3, and was referred to as the fugacity capacity of surfaces:

$$z.sur = \frac{z.air \times 82{,}500}{vapor^{0.65}} \quad (27)$$

where:

$z.sur$ = fugacity capacity of surface; molar density on surface [mol/Pa/m^3]
$vapor$ = vapor pressure [Pa]

Particle-air. The particle-air partition coefficient is given by (Bennett and Furtaw 2004) in the form of base 10 logarithms. The 0.74 in the below equation reflects the fraction of organic matter that is carbon.

$$\log(K_p) = \log(K_{oa}) + \log\left(\frac{f.carb}{0.74}\right) - 11.91 \quad (28)$$

$$K_p = K_{oa} \times \left(\frac{f.carb}{0.74}\right) \times 10^{-11.91} \quad (29)$$

where:

K_p = particle-air partition coefficient [m^3/mg]
K_{oa} = octanol-air partition coefficient [-]
$f.carb$ = fraction of organic matter that is carbon [-]

The octanol-air partition coefficient is given by:

$$K_{oa} = \frac{K_{ow} \times R \times T}{H} \quad (30)$$

$$H = \frac{vapor}{solub} \quad (31)$$

where:

K_{oa}	=	octanol-air partition coefficient [-]
K_{ow}	=	octanol-water partition coefficient [-]
R	=	ideal gas constant, 8.314 [Pa-m^3/mol]
T	=	temperature [K]
H	=	Henry's law constant [Pa-m^3/mol-K]
$vapor$	=	vapor pressure [Pa]
$solub$	=	solubility [mol/m^3]

Combining the above equations with that of the fugacity of pure air (equation 15) gives the particle-air partition coefficient for small and large particles, where the difference between the two is due to differences in $f.carb$.

$$sm.kp = \frac{(1.6625 \times 10^{-12}) \times K_{ow} \times sm.carb.f \times solub}{vapor \times z.air} \quad (32)$$

$$lg.kp = \frac{(1.6625 \times 10^{-12}) \times K_{ow} \times lg.carb.f \times solub}{vapor \times z.air} \quad (33)$$

where:

$sm.kp$	=	particle-air partition coefficient for small particles [m^3/mg]
$lg.kp$	=	particle-air partition coefficient for large particles [m^3/mg]

5.2.6 Particle masses

Each of the air and surface compartments may have a mass of small particles and also a mass of large particles. These masses are determined from the particle loadings and the compartment sizes. The loadings are input variables that depend only on the type of compartment and not on its location. The formulas for particle variables are:

$$vol.air = area.sur \times height \quad (34)$$

$$sm.mass.air = sm.load.air \times vol.air \quad (35)$$

$$lg.mass.air = lg.load.air \times vol.air \quad (36)$$

$$sm.mass.sur = sm.load.sur \times area.sur \quad (37)$$

$$lg.mass.sur = lg.load.sur \times area.sur \quad (38)$$

$$ug.mol = 10^6 \times molwt \text{ (g/mol)} \quad (39)$$

where:

$vol.air$	=	air volume in house [m^3]
$sm.mass.air$	=	small particle mass in air [mg]

$lg.mass.air$ = large particle mass in air [mg]
$sm.mass.sur$ = small particle mass on surfaces [mg]
$lg.mass.sur$ = large particle mass on surfaces [mg]
$ug.mol$ = conversion factor from g/mol to µg/mol

The $ug.mol$ variable is a unit conversion factor, used because some equations (see below) were developed for chemical masses expressed in moles, but the S2D code always uses chemical masses in micrograms (mg).

5.2.7 Cleaning rates

Cleaning includes all mechanisms that remove particles without having them enter another specific compartment. For floors, cleaning mechanisms include sweeping, mopping, and vacuuming. For air, cleaning includes dust filters in HVAC systems and (in some houses) electrostatic air filters. Particles removed by cleaning take their associated chemical content with them and it permanently leaves the system.

There are four cleaning rates, randomly sampled from the input distributions (in the house properties function), that correspond to large and small particles in air, and large and small particles on surfaces. Cleaning rates do not depend on the chemical, only on the compartment and particle size, so there are always four rates per house.

Particle flow balance requires that the total inflow equals the total outflow for each compartment. Separate balances are required for small and large particles since their flow rates generally differ. For surfaces, the specified inflow is deposition, while the specified outflows are resuspension and cleaning. For air, the specified inflow is resuspension, while the outflows are deposition and cleaning. These rates are sampled from distributions, so while the specified outflows usually exceed the specified inflows, occasionally the random sampling will imply a negative particle source rate. In such cases, the appropriate cleaning removal rate is increased to the point where the outflow (including cleaning) equals the inflow, and the implied particle source strength is zero.

To determine the potential adjustments needed to the cleaning rates in order maintain particle mass balance, the following constraints shown below for surface and air must be followed. While the equations for air and surface are different, the equations for small and large particles (within each compartment) have the same form, but refer to size-specific variables. The following discussion below is for small particles. However, the same questions apply to large particles, with each prefix “sm” replaced by “lg”.

Surface. For small particles on surfaces, the mass added to the surface is due to deposition of air particles. The rate and corresponding fractional rate, which is calculated by dividing by the surface loading, is given by:

$$add = sm.depos \times sm.load.air \quad (40)$$

$$frac.add = \frac{add}{sm.load.sur} \quad (41)$$

where:

add	=	rate of mass added to surfaces [mg/m^2/day]
$frac.add$	=	fractional rate of mass added to surfaces [1/day]
$sm.depos$	=	small particle deposition rate, from air to surface [m/day]
$sm.load.air$	=	small particle loading in air [mg/m^3]
$sm.load.sur$	=	small particle loading on surfaces [mg/m^2]

The mass removal rate, and corresponding fractional rate, by resuspension are given by:

$$rem = sm.resus \times sm.load.sur \quad (42)$$

$$frac.rem = \frac{rem}{sm.load.sur} \quad (43)$$

where:

rem	=	rate of mass removed from surfaces by resuspension [mg/m^2/day]
$frac.rem$	=	fractional rate of mass removed from surfaces by resuspension [1/day]
$sm.resus$	=	small particle resuspension rate, from surface to air [1/day]
$sm.load.sur$	=	small particle loading on surfaces [mg/m^2]

The particle balance requirement is that:

$$frac.add \leq frac.rem + sm.clean.sur \quad (44)$$

where:

$sm.clean.sur$	=	rate at which small particles are removed from surfaces by cleaning [1/day]

As indicated above, the inequality in equation 44 reflects the possibility of clean particles being added (to the left side) through human activities. However, if too many particles are added, the right side may be insufficient to remove them. In these cases, the cleaning term is increased until equality is reached. This is a conservative assumption because in practice, the human source term will never be zero, so the cleaning rate must be larger still.

Combining the above equations results in:

$$sm.clean.sur \geq \frac{sm.depos \times sm.load.air}{sm.load.sur} - sm.resus \quad (45)$$

The cleaning rates from surfaces are sampled from the input distributions but then constrained to force particle mass balance as shown above.

Air. For air, the equations are slightly different from those used for surfaces. Although there is air exchange with the outdoors, it is assumed that the particle density is the same indoors and outdoors, so there is no net flow. The equations for rate and corresponding fractional rate of mass addition and removal is given by:

$$add = sm.resus \times sm.mass.sur \quad (46)$$

$$frac.add = \frac{add}{sm.mass.air} \quad (47)$$

$$rem = sm.depos \times sm.load.air \times area.sur \quad (48)$$

$$frac.rem = \frac{rem}{sm.mass.air} \quad (49)$$

where:

add	=	rate of mass added to air [mg/day]
$frac.add$	=	fractional rate of mass added to air [1/day]
rem	=	rate of mass removed from air [mg/day]
$frac.rem$	=	fractional rate of mass removed from air [1/day]
$sm.resus$	=	small particle resuspension rate, surface to air [1/day]
$sm.mass.sur$	=	small particle mass on surfaces [mg]
$sm.mass.air$	=	small particle mass in air [mg]
$sm.depos$	=	small particle deposition rate, from air to surface [m/day]
$sm.load.air$	=	small particle loading in air [mg/m^3]
$area.sur$	=	total floor area [m^2]

Substituting equations 46-49 into the overall particle balance, which holds true for both surfaces and air, the constraint that must be upheld is:

$$sm.clean.air \geq \frac{(sm.resus \times sm.mass.sur - sm.depos \times sm.load.air \times area.sur)}{sm.mass.air} \quad (50)$$

5.2.8 Chemical flows

The six dynamic flows from Figure 2 that are calculated in the chemical flows function are described below.

The cleaning rate constants for particles in air are given below. As a fraction of the airborne chemical is bound to small particles, the cleaning (removal) efficiency for small particles is reduced by this factor. A similar reduction occurs for large particle cleaning. Note the chemical vapor form cannot be cleaned in this way. The overall cleaning rate is the sum of the two particle terms. If one happens to be larger than the other, the model assumes that the chemical quickly repartitions between the small and large particles (and the vapor form), to re-establish the same fugacity in each phase.

$$sm.cln.air = sm.clean.air \times \frac{sm.zv.air}{zv.air} \quad (51)$$

$$lg.cln.air = lg.clean.air \times \frac{lg.zv.air}{zv.air} \quad (52)$$

$$cln.air = sm.cln.air + lg.cln.air \quad (53)$$

where:

$sm.cln.air$	=	cleaning rate for small particles in air [1/day]
$lg.cln.air$	=	cleaning rate for large particles in air [1/day]
$cln.air$	=	overall cleaning rate in air [1/day]
$\frac{sm.zv.air}{zv.air}$	=	fraction of the airborne chemical bound to small particles [-]
$\frac{lg.zv.air}{zv.air}$	=	fraction of the airborne chemical bound to large particles [-]

The cleaning rate constants for particles from surfaces (by vacuuming, sweeping, or mopping) follow the same form as that for air. It is assumed that such cleaning does not remove chemical that is embedded into the flooring material.

$$sm.cln.sur = sm.clean.sur \times \frac{sm.zv.sur}{zv.sur} \quad (54)$$

$$lg.cln.sur = lg.clean.sur \times \frac{lg.zv.sur}{zv.sur} \quad (55)$$

$$cln.sur = sm.cln.sur + lg.cln.sur \quad (56)$$

where:

$sm.cln.sur$	=	cleaning rate for small particles on surfaces [1/day]
$lg.cln.sur$	=	cleaning rate for large particles on surfaces [1/day]
$cln.sur$	=	overall cleaning rate for surfaces [1/day]

Particle deposition onto surfaces is given by the summation of small and large particle deposition:

$$sm.dep = area.sur \times sm.load.air \times sm.depos \times \frac{sm.cap}{zv.air} \quad (57)$$

$$lg.dep = area.sur \times lg.load.air \times lg.depos \times \frac{lg.cap}{zv.air} \quad (58)$$

$$dep = sm.dep + lg.dep \quad (59)$$

where:

$sm.dep$	=	deposition on floor by small particles [1/day]
$lg.dep$	=	deposition on floor by large particles [1/day]

dep = total deposition on floor [1/day]

Particle resuspension from surface to air is given by:

$$sm.res = sm.mass.sur \times \frac{sm.resus}{zv.sur} \quad (60)$$

$$lg.res = lg.mass.sur \times \frac{lg.resus}{zv.sur} \quad (61)$$

$$res = sm.res + lg.res \quad (62)$$

where:

$sm.res$ = resuspension by small particles [1/day]
$lg.res$ = resuspension by large particles [1/day]
res = total resuspension [1/day]

The chemical flow between air and surfaces due to diffusion is calculated using the diffusive transfer factor, which is adapted from (Bennett and Furtaw 2004) by blending two regressions, similar to equation X for $z.sur$. The overall diffusion is the minimum value from the two diffusion terms below:

$$yaf1 = \frac{diffus.air \times z.air}{thick.bou} \quad (63)$$

$$yaf2 = \frac{0.0135}{vapor^{0.32}} \quad (64)$$

$$yaf = \min(yaf1, yaf2) \quad (65)$$

where:

$yaf1$ = first diffusion term [mol/m^2-Pa-day]
$yaf2$ = second diffusion term [mol/m^2-Pa-day]
yaf = overall diffusion [mol/m^2-Pa-day]

and the diffusion from air to floor and from floor to air is given by:

$$diff.air = \frac{yaf \times area.sur \times ug.mol}{zv.air} \quad (66)$$

$$diff.sur = \frac{yaf \times area.sur \times ug.mol}{zv.sur} \quad (67)$$

where:

$diff.air$ = diffusion from air to floor [1/day]
$diff.sur$ = diffusion from floor to air [1/day]

5.3 Evaluation of affected skin area: eval.pucs.area()

This function determines the affected skin areas for each PUC. The data for determining these areas comes from the skin areas input file. All values are fractions of the total skin area. An overall fraction is given on the input file, which is interpreted as a mean value. Interpersonal variance is determined separately for hands and body, given as “high”, “medium”, or “low”. The actual skin areas are determined once per PUC (per household), and all are sampled from Beta distributions bounded by zero and one. The “hands” component is multiplied by 0.05 and the “body” component by 0.95, and then they are summed. The logic is that hands are typically 5% of a person’s total skin area.

Beta distributions have two shape parameters, called “c” and “d”. The mean of a Beta(c,d) is given by c/(c+d). The variance is given by $v = c\ d\ /((c+d)^2\ (c+d+1))$. The key point is that if both “c” and “d” are multiplied by the same factor, the mean is unchanged, but the variance decreases (if the factor is greater than one). For “high” variability, “c” is set to 1, for “medium”, “c” is set to 4, and for “low” variability, “c” is 12. Then “d” is chosen to give the correct mean (that is, d = c/mean-c). For each PUC, “c” and “d” are evaluated separately for each household.

Input

pucs	only those PUCs that are also part of the house diary (for any specific house being evaluated in the loop over houses), with related information including the PUC code, product type, a binary code for indoor/outdoor product, handling time, mass, product code, met value, and a binary tag for whether the product is a spray type
skin.areas	identifies which body parts are exposed to a PUC during use, per PUC; fraction of the total skin area that is associated with dermal contact on the body part specified is provided for both adults and children, as well as an associated variability.
q	randomly sampled probabilities for house, PUC and chemical variables for the specific household; these percentiles are used in randomly sampling variable values from probability distributions.

Output

pucs.areas	information on the fraction of the total body surface area that will be exposed during its use, along with other PUC specific information including the PUC code, product type, a binary code for indoor/outdoor product, handling time, mass, product code, met value, and a binary tag for whether the product is a spray type.

5.4 Evaluation of persons in household: list.persons()

This function details all the persons in this household.

Input

One record from the pophouse.csv input file

Output

A data table with one record for each person in the household (up to 20), with variables sex, age, primary, basal.vent, and BSA.

primary	value of 1 for the person whose exposure is being tracked, 0 for others in the household
basal.vent	base level breathing ventilation rate (m^3/day)
BSA	body surface area (cm^2)

5.5 Evaluation of prime individual properties: eval.prime()

This function determines specific personal variables for the primary individual in each household.

The primary individual in each household is the one whose exposure is being evaluated; other individuals in the household may contribute via their own product use to the indirect exposure component of the primary individual's exposure, however exposure of the other household members themselves is not evaluated. The primary household member bears no relation to the head of the household, and may be a minor. The variables evaluated are:

hand.wash	average number of hand washing events per day
hand.mouth	hand-to-mouth rate transfer (1/hr)
basal.vent	basal breathing ventilation rate (m^3/day)

5.6 Compilation of PUC information: eval.puc.wipe.rinse()

This function merges the PUC information with the removal fractions.

Input

The puc.types and compart.fracs R objects

Output

A data table with values for each PUC in the run for the following variables:

Fhands	The fraction of product mass on the skin going to the hands
FBody	The fraction of product mass on the skin going to the body
Frinseh	The fraction of hand loading rinsed off at end of product use
Frinseb	The fraction of body loading rinsed off at end of product use
Fwipeh	The fraction of hand loading wiped off at end of product use
Fwipeb	The fraction of body loading wiped off at end of product use
Frinses	The fraction of surface loading rinsed off at end of product use
Fwipes	The fraction of surface loading wiped off at end of product use

Chemical mass that is rinsed off is added to the "drain" variable, a measure of the amount of chemical added to the wastewater treatment system due to a household's product use. Chemical mass wiped off is added to the "waste" variable, which measures the chemical component of solid waste which is due to a household's product use.

5.7 Evaluation of dermal rate constants: eval.dermal.rates()

For each chemical, the dermal rates function calculates the rate constants for the four competing chemical removal processes from the skin. The terms, equations, and approach used are described in detail below. A full discussion of competing physical removal processes can be found in (Isaacs, Glen et al. 2014).

Inputs

fug.cvars	chemical properties of each chemical
hp	specific house properties
prime	demographic information on the primary individual and exposure factors such as basal ventilation rate, skin surface area, hand washing, and hand to mouth transfer rates
pucs.areas	information on the fraction of the total body surface area that is exposed during PUC use, along with other PUC specific information including the PUC code, product type, a binary code for indoor/outdoor

	product, handling time, mass, product code, met value, and a binary tag for whether the product is a spray type
prod.chem	mass fractions of chemicals, the representative products and formulations, along with release fraction information
nc	number of chemicals being modeled in the current model run.
house.num	the house number (for aligning random number selection)

Outputs

dermal.rates	rate constants for the four competing chemical removal processes from the skin surface, plus the product layer thickness on the skin, for each PUC and for indirect contact

The dermal rates function determines the rate constants for the four competing chemical removal processes from the skin surface: absorption into the stratum corneum, evaporation into the air, hand-to-mouth transfer, and other removal (e.g., rubbing off, handwashing, transfer to other surfaces). In this version of the model, the rate constant for other removal was set to zero. Rate constants for hand-to-mouth transfer are based on results from a custom version of EPA's SHEDS-Multimedia model designed to predict soil and dust ingestion rates (Ozkaynak, Xue et al. 2011) (see Section 4.1.5).

The rate constants for absorption into the stratum corneum and evaporation into the air are calculated using the following equations described in (Ernstoff, Fantke et al. 2016). A key assumption is that the product applied to the skin can be modeled as an aqueous solution. Under this scenario, conventional two-film theory is used to model the steady-state mass transfer processes.

$$k_{sk,abs} = \left(\frac{h}{K_p} + \frac{h}{\varphi_w}\right)^{-1} \quad (68)$$

$$k_{sk,evap} = \left(\frac{h}{\varphi_a} + \frac{h}{\varphi_w}\right)^{-1} \quad (69)$$

where:

$k_{sk,abs}$	=	rate constant for absorption from skin surface into stratum corneum [h^{-1}]
$k_{sk,evap}$	=	rate constant for evaporation from skin surface to air [h^{-1}]
h	=	thickness of product layer on the skin [m]
K_p	=	skin permeation coefficient for aqueous solutions [m/h]
φ_w	=	water-side mass transfer rate [m/h]
φ_a	=	air-side mass transfer rate [m/h]

The product layer thickness on the skin is calculated using the following equations:

$$h = \frac{V_p}{A_{sk,aff}} \quad (70)$$

$$V_p = \frac{M_p \times f_{sk}}{\rho} \quad (71)$$

$$A_{sk,aff} = f_{aff} \times A_{sk} \quad (72)$$

where:

h	=	product layer thickness [m]
V_p	=	product volume [m^3]
$A_{sk,aff}$	=	affected skin area [m^2]
M_p	=	total mass of product per use [g]
f_{sk}	=	fractional release of chemical to skin [-]
ρ	=	product density [g/cm^3]
f_{aff}	=	fraction of skin in contact with the product [-]
A_{sk}	=	total skin area [m^2]

A minimum product layer thickness is required to prevent the rates from becoming excessively large. As a practical matter, the thickness "h" determined above is applicable only if it is appreciably larger than the standard thickness of the natural skin surface layer. This minimum is set to 1E-5 m, which is 10 microns.

The fraction of skin in contact with the product varies by PUC and differs between a child, defined as under 18 years of age, and an adult, defined as 18 years of age or older. For product density, a unit density of 1 g/cm^3 is assumed.

The skin permeation coefficient for aqueous solutions was provided by EPA and were calculated following the ten Berge model (ten Berge 2009):

$$K_p = \left(10^{-2.59 + 0.7318 \times logK_{ow} - 0.006832 \times MW} + \frac{0.043}{MW^{1.361}}\right) \times \left(\frac{\text{m}}{100\ \text{cm}}\right) \quad (73)$$

where:

K_p	=	skin permeation coefficient for aqueous solutions [m/h]
K_{ow}	=	octanol-water partition coefficient [-]
MW	=	molecular weight [g/mol]

The water-side mass transfer rate is estimated in (Ernstoff, Fantke et al. 2016) at normal skin temperature of 305 K (32°C) and is given as:

$$\varphi_w = 20.6 \times MW^{-0.4757} \quad (74)$$

where:

φ_w	=	water-side mass transfer rate [m/h]
MW	=	molecular weight [g/mol]

The air-side mass transfer rate is estimated by (Ernstoff, Fantke et al. 2016):

$$\varphi_a = v_{con,h} \times K_{aw} \quad (75)$$

$$K_{aw} = \frac{H_{c,T}}{R \times T} \quad (76)$$

$$H_{c,T} = H_c \times \exp\left[\frac{-\Delta H_{vap}}{R}\left(\frac{1}{T} - \frac{1}{298K}\right)\right] \quad (77)$$

where:

φ_a	=	air-side mass transfer rate [m/h]
$v_{con,h}$	=	transfer velocity due to air convection around the head [m/h]
K_{aw}	=	temperature adjusted air-to-water partition coefficient [-]
$H_{c,T}$	=	temperature adjusted Henry's law constant [J/mol]
R	=	ideal gas constant = 8.314 [J/K/mol]
T	=	absolute temperature [K]
H_c	=	standard temperature Henry's law constant at 298K [J/mol]
ΔH_{vap}	=	temperature independent enthalpy of vaporization (liquid-gas change) [J/mol]

The transfer velocity due to air convection around the head ($v_{con,h}$) is assumed to be 8 m/h. This was based on values for the head (Ernstoff, Fantke et al. 2016) and the human body (Weschler and Nazaroff 2012), which were estimated using two different methods and correspond to 9 m/h and 5-10 m/h, respectively.

The current version of the S2D module does not allow for temperature variation. The absolute temperature is set to be 298K, and therefore the temperature adjusted Henry's law constant is equal to the standard temperature Henry's law constant. For future versions, temperature variation can be taken into account using an estimated temperature independent enthalpy of vaporization, $\Delta H_{vap} \approx$ 50,000 J/mol.

The dermal rate constants are determined for each combination of product and chemical. The layer thickness "h" depends on the product and its usage parameters, and variables such as K_{aw} and $H_{c,T}$ depend on the chemical. An extra "product" called "Indirect" is included, which gives the rate constants for chemical picked up as indirect exposure.

6. Product use function: eval.use.data()

The Product Use function determines the mass of chemical in 11 different compartments at the end of the use phase. The terms, equations, and approach used are described in detail below.

Inputs

pucs	only those PUCs that are also part of the house diary (for any specific house being evaluated in the loop over houses), with related information, for example, the PUC code
prod.chem	mass fractions of chemicals, the representative products and formulations, along with release fraction information
fug.cvars	chemical properties of each chemical
dermal.rates	information on the rate constants for the four competing chemical removal processes from the skin surface: absorption into the stratum corneum, evaporation into the air, hand-to-mouth transfer, and other removal (e.g., rubbing off, handwashing, transfer to other surfaces)
puc.wipe.rinse	rinse-off and wipe-off fractions for each PUC being used by the household

Outputs

use.data	chemical masses in each of the 11 compartments for each of the three use phases shown in Figure 3, evaluated once per PUC; the code assumes that each member of the household uses each product similarly, so the same mass results apply to all household members

6.1 Product use categories, representative products, and formulations

The Product Use function is called once for each unique product use category (PUC) in each household product use diary (output from the Product Use Scheduler module). S2D currently considers over 300 unique PUCs, ranging from upholstery fabric cleaners to shampoos. For each PUC represented in the composition input file, there are multiple representative products, each with a different chemical make-up. Each representative product includes 100 different “formulations”. While all formulations for a representative product include the same set of chemicals, the quantified chemical mass fractions may differ between formulations (see Appendix A for details on the composition input file).

When a PUC is used by a given household, a representative product and formulation are randomly selected from the appropriate lists. Each representative product and formulation may contain, for example, 5-10 chemicals, but across all the possible representative product and formulation selections for one PUC, there may be over 100 different chemicals. An example of how representative products, formulations, and chemical mass fractions are related is shown below in Table 11.

Table 11. Example of representative products, formulations, and chemical mass fractions for the PUC corresponding to dry shampoos for removing hair oils.

Representative Product ID	Formulation #	Chemical DTXSID	Chemical Name	Chemical Mass Fraction
68375	0	DTXSID1026401	Isobutane	0.424
68375	0	DTXSID5026386	Propane	0.078
68375	0	DTXSID9020584	Ethanol	0.358
68375	1	DTXSID1026401	Isobutane	0.486
68375	1	DTXSID5026386	Propane	0.081
68375	1	DTXSID9020584	Ethanol	0.354
68375	…			
68375	99	DTXSID1026401	Isobutane	0.431
68375	99	DTXSID5026386	Propane	0.064
68375	99	DTXSID9020584	Ethanol	0.360
100385	0	DTXSID9020584	Ethanol	0.15
100385	0	DTXSID5026386	Propane	0.15
100385	0	DTXSID1026401	Isobutane	0.7
100385	0	DTXSID6023810	Ferene triazine	0.002
100385	0	DTXSID8020204	tert-Butyl alcohol	0
100385	…			
100385	99	DTXSID9020584	Ethanol	0.15
100385	99	DTXSID5026386	Propane	0.15
100385	99	DTXSID1026401	Isobutane	0.7
100385	99	DTXSID6023810	Ferene triazine	0.002
100385	99	DTXSID8020204	tert-Butyl alcohol	0

For the remainder of this manual, the term “product” will be used to describe the representative product and formulation pair randomly selected by S2D for each household.

Common PUCs will be used many times, perhaps daily, and possibly in a unique manner each time. However, the assumption is made that a given person will use the same product in the same way every time it is used. Therefore, once the outputs for each product have been determined, these can be re-used every time the same product is re-used by the same individual.

6.2 Preparatory calculations

Prior to running the Product Use function, the following preparatory steps are required:

eval.prod.chem() produces a table of masses and compartment fractions for each PUC.

eval.release.times() generates a calendar of chemical releases.

eval.use.chem() gives the chemical masses released in total by each product use.

6.3 General approach to modeling product use

The Product Use function implements a 3-phased mass partitioning approach, as shown in Figure 3. There are 11 compartments that a chemical can partition into: indoor air, outdoor air, indoor surface (residential), outdoor surface, skin, gut, hair/nails, solid waste (*a priori* assumption per use for amount left in container), drain, in appliance (enclosed), and remains as solid product. The function calculates the chemical mass released to each of the 11 compartments at the end of each of the three "use phases" shown in Figure 3 which correspond to: start of product use, active use, and end of product use.

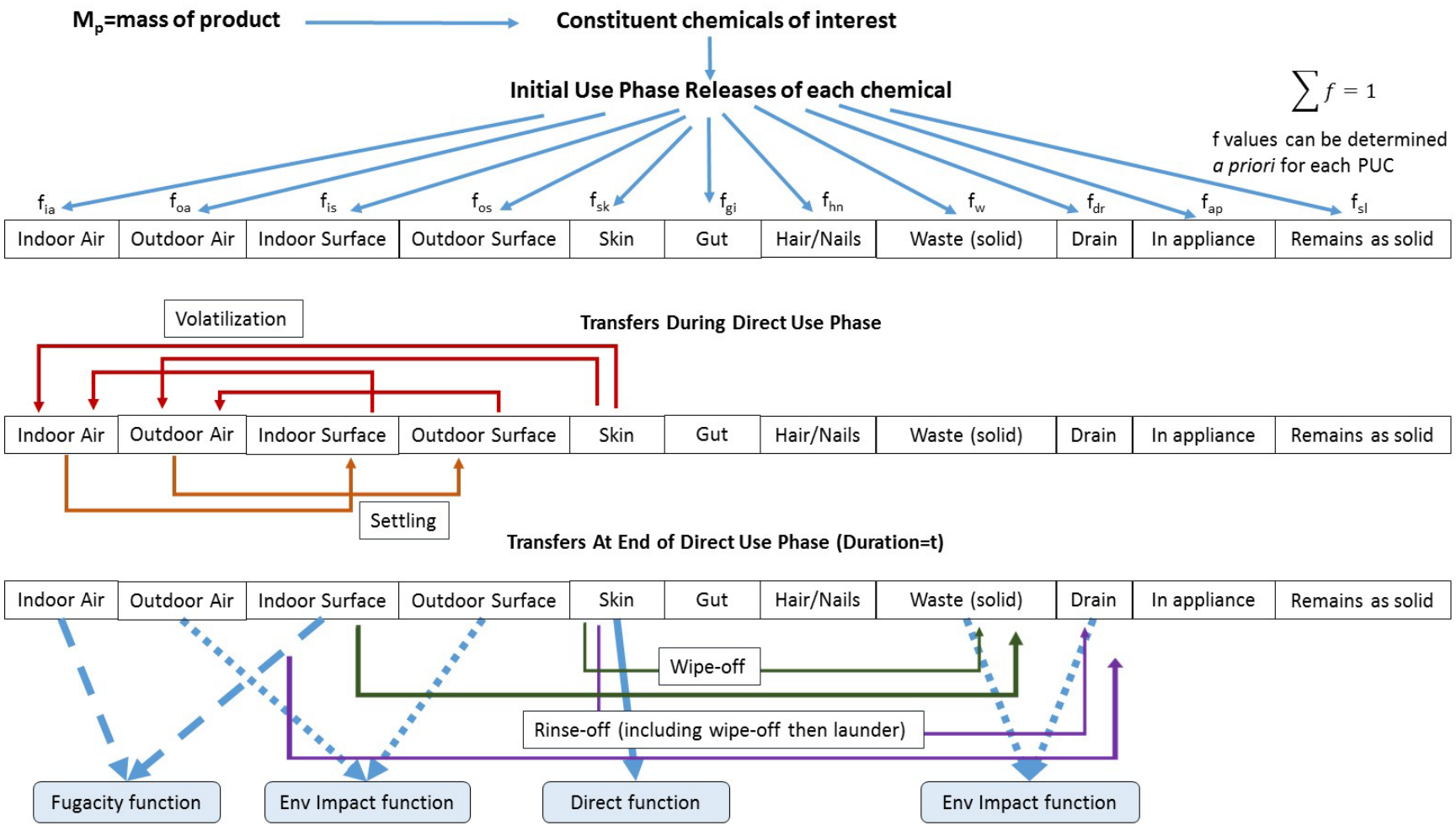

Figure 3. Mass partitioning approach for S2D exposure algorithms.

For products used in appliances such as washers, dryers, and dishwashers, the current version of the S2D module assigns chemical masses to the appliance compartment. Further handling of such chemicals will be dealt with in future versions of the S2D module.

6.4 Use Phase 1: Start of product use

Each time a product is used in a given household, the total mass of the product used in each instance is provided in the product use diaries output from the Product Use Scheduler for each household. The initial mass of each chemical in the product is calculated using the chemical mass fractions provided in the composition input file as follows:

$$M_c = f_c \times M_p \tag{78}$$

where:

M_p = total mass of product per use [mg]
M_c = initial mass of chemical in the product [mg]
f_c = chemical mass fraction in the product, specific to PUC brand and formulation [-]

For any given representative product and formulation for a PUC,

$$\sum_{i=1}^{n} f_{c,i} = 1 \tag{79}$$

where:

$f_{c,i}$ = chemical mass fraction in the representative product for chemical *i* [-]
n = number of chemicals in the formulation

Each chemical is then tracked separately and undergoes partitioning into the 11 compartments shown in Figure 3, and listed in Table 12 based on their fractional release variables. For each chemical, the sum of their fractional release variables is equal to 1, as shown below:

$$\sum_{j=1}^{11} f_j = 1 \tag{80}$$

where:

f_j = fractional release of chemical into compartment *j* [-]
j = one of 11 compartments shown in Figure 2 [-]

Please note that though the 'f' variable is common, $f_{c,i}$ and f_j defined in equations 79 and 80 represent different variables.

The mass of chemical in each compartment at the end of Use Phase 1 is then calculated as:

$$M_{c,j,1} = f_j \times M_c \quad (81)$$

where:

$M_{c,j,1}$ = mass of chemical in each compartment at end of Use Phase 1 [mg]
M_c = initial mass of chemical in the product [mg]
f_j = fractional release of chemical into compartment *j* [-]

Table 12. Fractional release variables for each compartment.

Fractional Release Variable	Compartment
f_{ia}	Indoor air
f_{is}	Indoor surface
f_{oa}	Outdoor air
f_{os}	Outdoor surface
f_{sk}	Skin
f_{gi}	Gut
f_{hn}	Hair/Nail
f_{dr}	Drain
f_{ws}	Waste (solid)
f_{ap}	In appliances
f_{sl}	Remains as solid

The fractional release variables apply to all chemicals in a given PUC. In the example of dry shampoos for removing hair oil shown in Table 11, the fraction of chemical released to hair would be the same for isobutene, propane, ethanol, and ferene triazine.

In addition, S2D considers the fractional release variables for each compartment to be the same for all PUCs that are used in the same manner. For example, all PUCs that are classified as "aerosols for application to non-dermal body (hair/nails)" will have the same fractional release to hair and the same fractional release to waste. The over PUCs assessed in the current version of the S2D module have all been classified into one of 30 "product type categories" based on how each PUC is used, with a 31st category for PUCs that are not assessed in the current version of the S2D module. Table 13 lists the 30 categories currently used, as well as some example PUCs for each category.

Table 13. Product type categories used for the mass partitioning approach.

Category	Category Description	Example PUCs
ABS	Aerosols for application to body surfaces	• Deodorants and antiperspirants[a] • Insect repellants for skin[a]
AGI	Aerosols for application to nose, mouth, or lips	• None considered in this version
AHN	Aerosols for application to non-dermal body (hair/nails)	• Dry shampoos for removing hair oils • Temporary hair colors and dyes[a]
AIA	Aerosols for application to indoor air	• Home air fresheners (including gel) [a] • Candles
AIS	Aerosols for application to indoor surfaces	• General purpose repair adhesives • Fabric starches
AOA	Aerosols for application to outdoor air	• Air fresheners for car interiors • Insecticides for exterior use[a]
AOS	Aerosols for application to outdoor surfaces	• None considered in this version
BAT	Soluble products added to bath water	• Bath oils or oil-filled beads • Bubble baths
DAP	Dusts or powders for application within appliances	• Dryer fabric softener sheets • Detergents for automatic dishwashers[b]
DBS	Dusts or powders for application to body surfaces	• Cheek blushes, bronzers, and rouges • Baby powder (specifically marketed for babies)
DGI	Dusts or powders for application to nose, mouth, or lips	• None considered in this version
DHN	Dusts or powders for application to non-dermal body (hair/nails)	• None considered in this version
DIS	Dusts or powders for application to indoor surfaces	• Carpet deodorizers • Potting soil and vermiculite
DOS	Dusts or powders for application to outdoor surfaces	• Lawn fertilizers • Mulches
LAP	Liquids, lotions, or gels for application within appliances	• Laser printer toners • Laundry detergents and soaps
LBS	Liquids, lotions, or gels for application to body surfaces	• Baby wipes • Eyelash mascara
LDR	Liquids, lotions, or gels for application to drains	• Septic system treatment products • Drain openers or digesters
LGI	Liquids, lotions, or gels for application to nose, mouth, or lips	• Denture adhesives • Toothpastes and dentrifices
LHN	Liquids, lotions, or gels for application to non-dermal body (hair/nails)	• Chemical hair relaxers • Nail polish
LIS	Liquids, lotions, or gels for application to indoor surfaces	• Paint of lacquer thinners • Pens and markers containing liquid or gel ink
LOS	Liquids, lotions, or gels for application to outdoor surfaces	• Auto, engine, and brake degreasers • Paint and finish strippers
LSH	Liquids, lotions, or gels for application to indoor surfaces with hands	• Non-edible finger paints
SBS	Sprays (pump) for application to body surfaces	• Antibacterial hand sanitizers • Body oils
SGI	Sprays (pump) for application to nose, mouth, or lips	• Antiseptic and dental mouthwashes
SHN	Sprays (pump) for application to non-dermal body (hair/nails)	• Dry shampoos for removing hair oils[a] • Hair styling products

Category	Category Description	Example PUCs
SIA	Sprays (pump) for application to indoor air	• None considered in this version
SIS	Sprays (pump)s for application to indoor surfaces	• Upholstery fabric cleaners • Glass and window cleaners[a]
SOA	Sprays (pump) for application to outdoor air	• None considered in this version
SOL	Solid formulations	• Cat litters • Children's play dough
SOS	Sprays (pump) for application to outdoor surfaces	• Chemical animal repellents[a] • Fungicides
XXX	Not for evaluation in 2017	• Algaecidal products for pools, hot tubs, and spas • Liquid products for glazing craft pottery

[a]: spray or aerosol formulation specified
[b]: powder formulation specified

Sprays. For PUCs that are sprays, an additional particle settling step is included in the initial product use phase (Use Phase 1) to differentiate between the amount of chemical that remains in the air, and is therefore available for inhalation during the product use phase (Use Phase 2), and the amount of chemical that settles to surfaces. In a study that examined particle sizes and settling times for aerosolized particles, Schwarz and Koch (Schwarz and Koch 2017) studied the mass fraction released to air for respirable and thoracic particle sizes for a range of hair sprays. Based on the results for "hand-triggered pump sprays – household product" and "propellant sprays", the Product Use function assumes a mass fraction of 0.1 and 0.3 for respirable and thoracic particle sizes, respectively. The remaining fraction of aerosolized particles from sprays (equal to 0.6) is assumed to immediately settle onto surfaces. Using this settling fraction, the mass of chemical for indoor air, indoor surface, outdoor air, and outdoor surface, at the end of Use Phase 1, for sprays, is given as:

$$M_{c,ia,sprays,1} = M_{c,ia,1,0} - 0.6 \times M_{c,ia,1,0} \quad (824)$$

$$M_{c,is,sprays,1} = M_{c,is,1,0} + 0.6 \times M_{c,ia,1,0} \quad (83)$$

$$M_{c,oa,sprays,1} = M_{c,oa,1,0} - 0.6 \times M_{c,oa,1,0} \quad (84)$$

$$M_{c,os,sprays,1} = M_{c,os,1,0} + 0.6 \times M_{c,oa,1,0} \quad (85)$$

where:

$M_{c,j,sprays,1}$ = mass of chemical in compartment *j* for sprays at the end of Use Phase 1 [mg]
$M_{c,j,1,0}$ = mass of chemical in compartment *j* for sprays at the beginning of Use Phase 1 [mg]
j = one of 11 compartments shown in Figure 3 [-], with specific values of *j* = *ia*, *is*, *oa* and *os* in Equations 82-85, respectively.

The equations shown above assume that the respirable and thoracic fractions (which account for 0.4 of aerosolized particles and are not differentiated in the Product Use function) remain suspended in the air at the end of Use Phase 1. This assumption is supported by Schwarz and Koch (Schwarz and Koch 2017),

who found that the settling times for both respirable and thoracic particles were 250 seconds (~4 minutes) under conditions of slight ventilation.

It is important to note that for the Product Use function, particle settling is assumed to only apply for PUCs that are sprays. For PUCs that are aerosols, a fraction of the chemical mass will be released to indoor (or outdoor) air; however, it is assumed that no settling occurs for aerosols during any use phase of the Product Use function because aerosol products release a mist or vapor that contain fine particles with no appreciable settling during the relatively short active use and end of use phases.

6.5 Use Phase 2: During product use

During product use phase (shown as the second use phase in Figure 3), chemical transfers can occur between the compartments. The primary transfers that occur include transfers between the skin and air compartments, and transfers between surfaces and air. These transfers depend on the physiochemical properties of each chemical, so the flows are chemical-specific. The current version of the S2D module considers transfer between five compartments (indoor air, indoor surface, outdoor air, outdoor surface, skin) but is adaptable to accommodate additional inter-compartmental transfers if determined appropriate during continued development.

Transfers from skin (or indoor/outdoor surface) to air occur as the chemical volatilizes from the skin (or indoor/outdoor surface). The rate of volatilization is determined by assuming that volatilization follows a first order reaction as given by:

$$r_{vol} = k \times M_c \quad (86)$$

where:

r_{vol} = rate of volatilization from skin/surface to air [mg/min]
k = volatilization rate constant [min^{-1}]
M_c = mass of chemical on skin/surface [mg]

For chemical volatilization from skin to air, the rate constant is calculated and explained in the Dermal Rates function (Section 5.7.1). For transfer from indoor/outdoor surfaces to air, the rate constant is estimated from the physical properties of the chemical and an empirical relationship developed by Chinn (Chinn 1981) for the time required for 90% of a pure chemical film to evaporate:

$$k_{sur,evap} = \frac{\ln(10)}{t_{0.90}} \quad (87)$$

$$t_{0.90} = \frac{145}{(MW \times VP)^{0.9546}} \quad (88)$$

where:

$k_{sur,evap}$ = volatilization rate constant from surface to air [min^{-1}]
$t_{0.90}$ = time required to evaporate 90% of the chemical [min]

MW = molecular weight of chemical [g/mol]
VP = vapor pressure of chemical [mm Hg]

The mass of chemical transferred from skin or surface to air is then given by:

$$M_{c,j,2,transfer} = M_{c,j,2,0} - M_{c,j,2} = M_{c,j,2,0} \times (1 - exp^{-k \times t}) \quad (89)$$

where:

$M_{c,j,2,transfer}$ = mass of chemical transferred from compartment *j* (skin or surface) to air during Use Phase 2 [mg]
$M_{c,j,2,0}$ = mass of chemical in compartment *j* (skin or surface) at beginning of Use Phase 2 [mg]
$M_{c,j,2}$ = mass of chemical remaining in compartment *j* (skin or surface) at end of Use Phase 2 [mg]
j = compartment corresponding to indoor surface (is), outdoor surface (os), or skin (sk) [-]
k = volatilization rate constant from skin ($k_{sk,evap}$) or surface ($k_{sur,evap}$) to air [min^{-1}]
t = duration of active PUC use [min]

Accounting for chemical transfer between compartments, the mass of chemical in the affected compartments at the end of the active use phase can be calculated using equations 90-94. Depending on whether the product is used indoors or outdoors, only the relevant equations are used in the S2D code (e.g., if the product is used outdoors, only equations 92, 93, and 94 are used). The remaining compartments experience no change in chemical mass during the active use phase and therefore the mass at the end of Use Phase 2 remains the same as the mass at the beginning of Use Phase 2.

$$M_{c,ia,2} = M_{c,ia,2,0} + (M_{c,is,2,0} \times (1 - e^{-k_{sur,evap}t})) + (M_{c,sk,2,0} \times (1 - e^{-k_{sk,evap}t})) \quad (90)$$

$$M_{c,is,2} = M_{c,is,2,0} \times e^{-k_{sur,evap}t} \quad (91)$$

$$M_{c,oa,2} = M_{c,oa,2,0} + (M_{c,os,2,0} \times (1 - e^{-k_{sur,evap}t})) + (M_{c,sk,2,0} \times (1 - e^{-k_{sk,evap}t})) \quad (92)$$

$$M_{c,os,2} = M_{c,os,2,0} \times e^{-k_{sur,evap}t} \quad (93)$$

$$M_{c,sk,2} = M_{c,sk,2,0} \times e^{-k_{sk,evap}t} \quad (94)$$

where:

$M_{c,ia,2}$ = mass of chemical in indoor air at end of Use Phase 2 [mg]
$M_{c,is,2}$ = mass of chemical on indoor surfaces at end of Use Phase 2 [mg]
$M_{c,oa,2}$ = mass of chemical in outdoor air at end of Use Phase 2 [mg]
$M_{c,os,2}$ = mass of chemical on outdoor surfaces at end of Use Phase 2 [mg]
$M_{c,sk,2}$ = mass of chemical on skin at end of Use Phase 2 [mg]
$M_{c,j,2,0}$ = mass of chemical in compartment *j* at beginning of Use Phase 2 [mg]
j = indoor air (ia), indoor surface (is), outdoor air (oa), outdoor surface (os), or skin (sk) [-]

$k_{sur,evap}$ = volatilization rate constant from surface to air [min^{-1}]
$k_{sk,evap}$ = volatilization rate constant from skin to air [min^{-1}]
t = duration of active PUC use [min]

Particle settling. The current version of the S2D module does not assume any particle settling from sprays or other PUCs during the active use phase. However, future versions of the module may include terms that account for settling from products during the active use phase. In such an instance, the indoor/outdoor air concentration would decrease due to these transfers and the mass of chemical on surfaces would increase.

6.6 Use Phase 3: End of product use

The third use phase captures the transfer processes that occur in the immediate duration following active product use. Some PUCs may be subject to wipe-off or rinse-off, which may remove them from the skin or possibly other surfaces. The chemical then moves to the solid waste (for wipe-off) or drain compartments (for rinse-off), both of which are captured in the Environmental Impact function (Section 10). Some chemical may be left behind on the skin, in which case the post-use exposure is evaluated by the Direct Exposure function (Section 8). Chemical left behind on indoor surfaces or in air becomes an input to the Fugacity function (Section 7).

For products that are subject to wipe-off or rinse-off, the fraction of the skin corresponding to hands and to the body is provided for each PUC, and the initial mass of chemical on hands and body can be calculated as:

$$f_{sk,hands} + f_{sk,body} = 1 \quad (95)$$

$$M_{c,hands,3,0} = f_{sk,hands} \times M_{c,sk,3,0} \quad (96)$$

$$M_{c,body,3,0} = f_{sk,body} \times M_{c,sk,3,0} \quad (97)$$

where:

$f_{sk,hands}$ = fraction of skin corresponding to hands [-]
$f_{sk,body}$ = fraction of skin corresponding to body [-]
$M_{c,sk,3,0}$ = mass of chemical on skin at beginning of Use Phase 3 before wipe-off and/or rinse-off [mg]
$M_{c,hands,3,0}$ = mass of chemical on hands at beginning of Use Phase 3 before wipe-off and/or rinse-off [mg]
$M_{c,body,3,0}$ = mass of chemical on body at beginning of Use Phase 3 before wipe-off and/or rinse-off [mg]

Wiping and rinsing off are physical processes with no reaction term (i.e., no rate constant needed) and these transfer processes are represented in S2D using chemical removal mass fractions. The fraction of chemical mass that is removed through wiping or rinsing off is disaggregated by hands, body, and surfaces. At the end of Use Phase 3, the resulting chemical mass left on the hands, body, skin, and

(depending on where the product is used, indoor or outdoor) surfaces after rinse-off and wipe-off is given by:

$$M_{c,hands,3} = M_{c,hands,3,0} - \left(f_{rinse,h} + f_{wipe,h}\right) \times M_{c,hands,3,0} \quad (98)$$

$$M_{c,body,3} = M_{c,body,3,0} - \left(f_{rinse,b} + f_{wipe,b}\right) \times M_{c,body,3,0} \quad (99)$$

$$M_{c,sk,3} = M_{c,hands,3} + M_{c,body,3} \quad (100)$$

$$M_{c,sur,3} = M_{c,sur,3,0} - \left(f_{rinse,s} + f_{wipe,s}\right) \times M_{c,sur,3,0} \quad (101)$$

where:

$M_{c,hands,3}$ = mass of chemical remaining on hands at end of Use Phase 3 after wipe-off and/or rinse-off [mg]
$M_{c,body,3}$ = mass of chemical remaining on body at end of Use Phase 3 after wipe-off and/or rinse-off [mg]
$M_{c,sk,3}$ = mass of chemical remaining on skin at end of Use Phase 3 after wipe-off and/or rinse-off [mg]
$M_{c,sur,3}$ = mass of chemical remaining on surfaces at end of Use Phase 3 after wipe-off and/or rinse-off [mg]
$M_{c,n,3,0}$ = initial mass of chemical at beginning of Use Phase 3 before wipe-off and/or rinse-off [mg]
n = hands, body, skin (sk), or surfaces (sur) [-]
$f_{rinse,n}$ = mass fraction of chemical removed by rinsing [-]
$f_{wipe,n}$ = mass fraction of chemical removed by wiping [-]

The chemical mass that is removed to solid waste through wipe off and to drain through rinse off is given by:

$$M_{c,waste,3} = M_{c,waste,3,0} + f_{wipe,h} \times M_{c,hands,3,0} + f_{wipe,b} \times M_{c,body,3,0} + f_{wipe,s} \times M_{c,sur,3,0} \quad (102)$$

$$M_{c,drain,3} = M_{c,drain,3,0} + f_{rinse,h} \times M_{c,hands,3,0} + f_{rinse,b} \times M_{c,body,3,0} + f_{rinse,s} \times M_{c,sur,3,0} \quad (103)$$

where:

$M_{c,waste,3}$ = mass of chemical removed to solid waste in Use Phase 3 through wipe-off and/or rinse-off [mg]
$M_{c,drain,3}$ = mass of chemical removed to drain in Use Phase 3 through wipe-off and/or rinse-off [mg]
$M_{c,n,3,0}$ = initial mass of chemical at beginning of Use Phase 3 before wipe-off and/or rinse-off [mg]
n = hands, body, surfaces (sur), waste, or drain [-]
$f_{rinse,n}$ = mass fraction of chemical removed by rinsing [-]
$f_{wipe,n}$ = mass fraction of chemical removed by wiping [-]

Sprays. For the case of spray PUCs, as noted previously, the non-respirable and non-thoracic sized particles, which are equal to 60% by mass, are assumed to settle immediately onto surfaces at the start of product use. The remaining 40% of aerosolized particles remain in the air during the active use phase. At the end of the active use phase, it is assumed that all particles in the indoor and outdoor air compartments settle onto surfaces. In the S2D module, this is modeled to occur at the beginning of Use Phase 3 (and not Use Phase 2) prior to wipe-off or rinse-off, in order to ensure non-zero values for the indoor and outdoor air compartments at the end of active use phase.

$$M_{c,ia,sprays,3,0} = M_{c,ia,sprays,2} - M_{c,ia,sprays,2} \quad (104)$$

$$M_{c,is,sprays,3,0} = M_{c,is,sprays,2} + M_{c,ia,sprays,2} \quad (105)$$

$$M_{c,oa,sprays,3,0} = M_{c,oa,sprays,2} - M_{c,oa,sprays,2} \quad (106)$$

$$M_{c,os,sprays,3,0} = M_{c,os,sprays,2} + M_{c,oa,sprays,2} \quad (107)$$

where:

$M_{c,j,sprays,3,0}$ = mass of chemical in compartment *j* for sprays at the beginning of Use Phase 3 [mg]

$M_{c,j,sprays,2}$ = mass of chemical in compartment *j* for sprays at the end of Use Phase 2 [mg]

j = one of 11 compartments shown in Figure 2 [-]

7. Fugacity function: fug.concs.an()

The fugacity function determines how the chemical concentration in the house air and on house surfaces change with time, after product use ceases. Chemicals may continue to be present for many days after use, or even until the simulation ends (i.e., after one year). The fugacity function is based on the SHEDS-Fugacity model, adapted for multiple product use at different times. This version has just two compartments (one for air and the other for surfaces). More compartments would allow for differences from room to room. However, this is not useful here because we do not have house layouts, we do not generally know which room the products are used in, and we do not know which room specific people are in at various times of the day. Hence, whole-house average concentrations are used instead. The activity diaries reliably indicate whether each person is in the house (or not) throughout the year.

Input

chem.release	a vector containing the amount of each chemical released on each hour of the year, to air and to surfaces
flows	vectors of hourly flow rates between compartments
indoor.hrs	a list of which hours have chemical releases, with hours ranging from 1 to 8736
indoor.gaps	a list of the intervals between releases, in hours

Output

A compound object called “fugs”, containing two parts:

fug.day	daily average chemical masses in air and on surfaces, as well as the amounts added daily to outdoor air (called “win” for “out the window”) and to waste (called “was”)
fug.hour	has the same variables as fug.day, bur reports hourly data (8736 values for each variable)

7.1 General overview

The S2D fugacity calculations are based on those in the SHEDS-HT exposure model (see supplement to Isaacs et al. (Isaacs, Glen et al. 2014)), which incorporated simplifications to the ten-compartment SHEDS-Fugacity model, which in turn was based on an indoor fugacity model as described in Bennett and Furtaw (Bennett and Furtaw 2004).

All four above-mentioned fugacity model versions have the following features in common:

Each version models a set of houses with chemical releases and dispersion.

The fugacity model must be run separately for each house, because both house properties and chemical releases differ.

With the exception of the original Bennett and Furtaw version, which only considered instantaneous chemical releases, later versions of SHEDS-Fugacity, SHEDS-HT, and the S2D Fugacity function include slow releases as well.

The fugacity model may contain any number of distinct compartments in a house; however, these compartments are considered to be either air or surface (that is, the chemical is either airborne or attached to solid materials, called “surfaces” for simplicity).

In S2D, the model used in the Fugacity function has only two compartments, generically called “a” or “air”, and “s” or “sur”. It may be expected that air concentrations remain non-uniform for a short time, compared to the length of the S2D simulation (one year at each house). Surface concentrations may never really equilibrate, but the model does not have details on where in the house a given person happens to be at all times. Hence, it is assumed that all house surfaces are contacted with equal frequency, which averages out (over many contacts) to the same value, whether the chemical is uniformly distributed, or not. Note that contact with chemical during or immediately after use, before it has left one’s personal bubble, is called “direct exposure” in S2D, and is modeled separately. The fugacity calculations support the indirect exposure, in which the chemical (or the person) has moved away from the location of product use, and then later re-encountered the chemical. For this purpose, the assumption of uniform surface concentrations is reasonable.

The S2D version uses instantaneous chemical releases. However, there may be several releases each day, sometimes amounting to thousands over the course of a year. In this respect, the S2D version is quite different from earlier versions of the fugacity model, which typically evaluated a single release in each house.

7.2 Fugacity model basics

Fugacity may be thought of as a chemical pressure. It measures the tendency of a chemical to leave the compartment in which it currently exists. The model consists of air and surface compartments connected to each other, and also connected to the outdoors. In this model, each compartment consists of three “phases”, which are bulk, small particles, and large particles. For the air compartment, the bulk phase is chemical in the vapor phase, while the small and large particles represent airborne dust containing particle-bound chemical. Surfaces are generally taken as synonymous with “floor” in this model, although table tops and other surfaces could be included. Vertical surfaces such as walls hold less dust and usually much less chemical than horizontal surfaces, so a simplifying assumption is that the available surface area is the total floor area of the house. If other surfaces were included, the same chemical mass would be spread out even thinner, which would reduce the exposure potential during contact with a particular area. This would be mitigated somewhat by having more surfaces available for contact, so the net effect would be unclear. The full SHEDS-fugacity model has ten compartments, including walls, so these could be reintroduced in S2D, if necessary. In S2D, the floor area is taken as the available surface area, and the air volume in the house is the product of the floor area and average room height.

Chemical moves between two air compartments by air exchange. In this model, air exchange always has equal volume in each direction. With just one indoor air compartment, the only air exchange is with the outdoors. Outdoor air is assumed to contain no chemicals of interest. However, the outdoor air is assumed to contain the same amount of particles as the indoor air. This is important because the model insists on particle balance, that is, the mass of particles in each compartment is constant in time.

Chemical moves from air to surfaces by particle deposition, or from surfaces to air by resuspension. Chemical may also transfer directly (by evaporation or condensation), without being bound to dust. Each compartment is assumed to be in internal equilibrium, meaning that its phases are always at the same fugacity as each other.

7.3 Steps in Source-to-Dose fugacity modeling

There are five steps in running the S2D fugacity calculations. First, the house properties are sampled from distributions in eval.house.props. These include not only physical size and air exchange, but dust levels and movement, and cleaning rates. The house properties are evaluated once per house, so they are assumed to remain fixed over time. The relevant chemical properties are similarly sampled in eval.chem.props. Next, the house and chemical properties are combined to determine the chemical flow rates in eval.flows. There are four flows (air-to-surface, surface-to-air, total losses from air, and total

losses from surfaces). Each is a fractional rate, which means the flow rate per unit time (measured in days) as a fraction of the chemical mass. For example, if the total loss rate from surfaces is 0.1, that means the time constant in the decay equation is 10 days. For air, the loss rate is generally well above one, which means that the time constant is much less than one day.

The fourth step is to evaluate the times and amounts of chemical releases into the indoor air and indoor surfaces in eval.chem.release. This is done on an hourly basis for the simulated year (that is, each chemical release is effectively instantaneous at a particular hour). The list of hours with non-zero releases is produced, as it informs the fugacity calculations when to reset the conditions. The final step is coded in eval.fug.concs.an, which evaluates the hourly time series of air and surface concentrations, taking into account the release times and the chemical flows.

7.4 Evaluation of differential equations for chemical flow

The hourly time series for mass of chemical in the air and in the surface is determined by solving the following differential equations:

$$\frac{dM_{air}}{dt} = (-a + b) \times M_{air} \tag{108}$$

$$\frac{dM_{sur}}{dt} = (c - d) \times M_{sur} \tag{109}$$

where:

$M_{air}(t)$	=	total mass of chemical in the house air as a function of time [mg]
$M_{sur}(t)$	=	total mass of chemical on surfaces as a function of time [mg]
a	=	total loss rate for air [1/day]
b	=	surface to air transfer [1/day]
c	=	air to surface transfer [1/day]
d	=	total loss rate for surfaces [1/day]

The rate constants for total loss rate for air, surface to air transfer, air to surface transfer, and total loss rate for surfaces are calculated in the chemical flows function. Since the unit time step of the fugacity calculations is taken to be one hour, the four flow rate constants are converted to units of (1/hr) by dividing each of the (1/day) rates by 24 at the start of the “eval.fug.concs.an” function.

To solve these differential equations, the S2D code puts these variables into matrix form, where the overall minus sign is taken out of the matrix by convention, to allow the matrix to be positive definite (meaning it has positive eigenvalues). If the initial values, $M_{air}(0)$ and $M_{sur}(0)$, are given, the values at any later time can be calculated.

$$\frac{d}{dt}\begin{pmatrix} M_{air} \\ M_{sur} \end{pmatrix} = -\begin{pmatrix} a & -b \\ -c & d \end{pmatrix}\begin{pmatrix} M_{air} \\ M_{sur} \end{pmatrix} \tag{110}$$

With more than two compartments (as in the original SHEDS-Fugacity model), it is necessary to solve numerically for the eigenvalues of the flow matrix, and then for the corresponding eigenvectors. An eigenvector is a distribution of chemical masses such that the proportions in each compartment remain fixed as time progresses. Each compartment undergoes exponential decay at a rate given by the corresponding eigenvalue.

Any initial mass distribution among the compartments may be expressed as a linear combination of the eigenvectors. As time progresses, each term decreases at the corresponding exponential decay rate. Note that some of the coefficients in the linear combination may be negative, which means that as time progresses, a smaller amount is being subtracted, which means the amount of chemical in the compartment increases. Eventually, the solution is dominated by the term with the smallest eigenvalue, (which decreases the slowest with time), and this eigenvector has all positive coefficients. Therefore, after some time all compartments continue to lose chemical until it is all gone.

In the S2D algorithm, there is generally not enough time for all the chemical to be lost. Chemical releases tend to occur very frequently, perhaps many times per day. The simulation covers 364 days. Every time a new release occurs, the Mair and Msur values must be readjusted. This also means recalculating the breakdown of these values into linear combinations of the eigenvectors. However, the eigenvalues and eigenvectors themselves are not altered by the addition of more chemical, so these only need to be evaluated once per house.

For the two compartments of air and surfaces considered in S2D, the eigenvalues and eigenvectors may be expressed directly as functions of the flow matrix. For the matrix $\begin{pmatrix} a & -b \\ -c & d \end{pmatrix}$, the eigenvalues are:

$$\lambda_1 = \frac{\left(a + d + \sqrt{a^2 + 4\,b\,c - 2\,a\,d + d^2}\right)}{2} \tag{111}$$

$$\lambda_2 = \frac{\left(a + d - \sqrt{a^2 + 4\,b\,c - 2\,a\,d + d^2}\right)}{2} \tag{112}$$

Both eigenvalues must be positive and λ_2 is smaller. Since the expression under the square root also appears in the eigenvalues, this is referred to as:

$$rterm = \sqrt{a^2 + 4\,b\,c - 2\,a\,d + d^2} \tag{113}$$

The eigenvalues specify the ratio of air to surfaces masses, but the overall scaling is arbitrary. With unit length eigenvectors v1 and v2, it may be shown that the breakdown of the initial air and surface masses into eigenvector components is as follows:

$$\begin{pmatrix} M_{air}(0) \\ M_{sur}(0) \end{pmatrix} = \begin{pmatrix} k_{1a} & k_{2a} \\ k_{1s} & k_{2s} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \tag{114}$$

The coefficients are:

$$k_{1a} = \frac{[2 \times b \times M_{air}(0) + (a - d - rterm) \times M_{sur}(0)] \times (a - d + rterm)}{4 \times c \times rterm} \quad (115)$$

$$k_{2a} = \frac{[2 \times b \times M_{air}(0) + (a - d + rterm) \times M_{sur}(0)] \times (d - a + rterm)}{4 \times c \times rterm} \quad (116)$$

$$k_{1s} = -\frac{[2 \times b \times M_{air}(0) + (a - d - rterm) \times M_{sur}(0)]}{2 \times rterm} \quad (117)$$

$$k_{2s} = \frac{[2 \times b \times M_{air}(0) + (a - d + rterm) \times M_{sur}(0)]}{2 \times rterm} \quad (118)$$

The chemical masses at a time "t" hours later are:

$$M_{air}(t) = k_{1a} \times e^{-\lambda_1 t} + k_{2a} \times e^{-\lambda_2 t} \quad (119)$$

$$M_{sur}(t) = k_{1s} \times e^{-\lambda_1 t} + k_{2s} \times e^{-\lambda_2 t} \quad (120)$$

As long as no new chemical releases occur, the same solution may be used, just increasing the time "t" by one hour at a time. The goal is to evaluate $M_{air}(t)$ and $M_{sur}(t)$ at all values of "t" from the beginning of the year ($t = 0$) to the end ($t = 364 \times 24$). Note that every chemical has its own time series.

If a new chemical release occurs, the M_{air} and M_{sur} for that hour, as given by the above equations, are incremented by the amounts released. This requires re-evaluating k_{1a}, k_{2a}, k_{1s}, k_{2s}, and resetting the time lag variable "t" to zero.

The releases for different chemicals may occur at different times. The current S2D module reevaluates all the k_{1a}, k_{2a}, k_{1s}, k_{2s} (for all chemicals) on all hours when any new chemical release occurs. This is not ideal, as any chemicals not released at that time can continue to use the previous values. This is a possible efficiency enhancement for the future.

The result of these calculations are values for $M_{air}(t)$ and $M_{sur}(t)$, at all hours "t" in the year. Note that these are chemical masses (in micrograms), not chemical concentrations, which are needed for exposure.

8. Direct Exposure function: eval.direct()

The Direct Exposure function calculates route-specific dermal, inhalation, and ingestion chemical exposures for the primary individual in each household due to sources that the primary individual uses directly. Note that in this usage, "primary" refers to the individual chosen by the RPGen module to have their exposure fully assessed, and is not an indicator of age or status. This does not include the contributions to exposure from the activities of other individuals in the house or the delayed exposure

from the primary individual's earlier activities (both of which are evaluated by the indirect exposure function). Daily direct exposure metrics are calculated by first calculating exposure per product use and then summing together the contributions from each product use over each day.

Inputs

d	all diary activity events for the primary individual in the household
use.data	chemical masses, with one dimension each for the number of PUCs being used by the household, the use phase, number of compartments to which the PUC releases chemical to, and the number of chemicals in the representative product and formulation that has been randomly chosen for the household for each PUC used
use.chem	total mass of each chemical released by each PUC's use in the household
pucs	only those PUCs that are also part of the house diary (for any specific house being evaluated in the loop over houses), with related information, for example, the unique PUC identifier code
dermal.rates	information on the rate constants for the four competing chemical removal processes from the skin surface: absorption into the stratum corneum, evaporation into the air, hand-to-mouth transfer, and other removal (e.g., rubbing off, handwashing, transfer to other surfaces)
compart.list	names of the 11 compartments that are being modeled as part of the mass partition approach
prime	demographic information on the primary individual and exposure factors such as basal ventilation rate, skin surface area, hand washing and hand to mouth transfer rates
puc.wipe.rinse	rinse-off and wipe-off fractions for each PUC being used by the household
chem.list	all chemicals
fug.cvars	chemical properties of each chemical
chem.totals	total annual household usage (mg) of each chemical

Outputs

direct	daily exposure metrics as defined in Table 2, including the dermal exposure ind.derm.exp (mg), dermal maximum loading ind.derm.max (mg/cm^2), dermal absorbed dose ind.derm.abs (mg), inhalation exposure ind.inhal.exp (mg/m^3), inhaled mass ind.inhal.mass (mg), maximum air concentration ind.inhal.max

(mg/m^3), inhaled mass of chemical absorbed ind.inhal.abs (mg), ingested chemical mass ind.ingest.exp (mg), and ingested chemical mass absorbed ind.ingest.abs (mg)

8.1 Overview of exposure routes

There are three direct exposure routes (dermal, inhalation, and ingestion) considered in S2D, as shown in Figure 4. All three direct exposure routes occur during the product active use and post-use phases. For simplicity, it is assumed that both the active use and post-use exposures take place on the same day the product use begins. From Figure 3, active use corresponds to Use Phase 2, while post-use corresponds to after Use Phase 3. The dermal exposure is unique in that once a chemical gets on the skin, there are three competing removal processes (four, if a product is used on the hands). The four dermal removal processes are absorption, evaporation, other removal (such as rubbing off, or transfer to other surfaces), and for the hands, there is also the possibility of hand-to-mouth transfer. Evaporation from the skin and hand-to-mouth transfer then lead to potential additional exposure by the inhalation and ingestion routes, respectively, as shown in Figure 4.

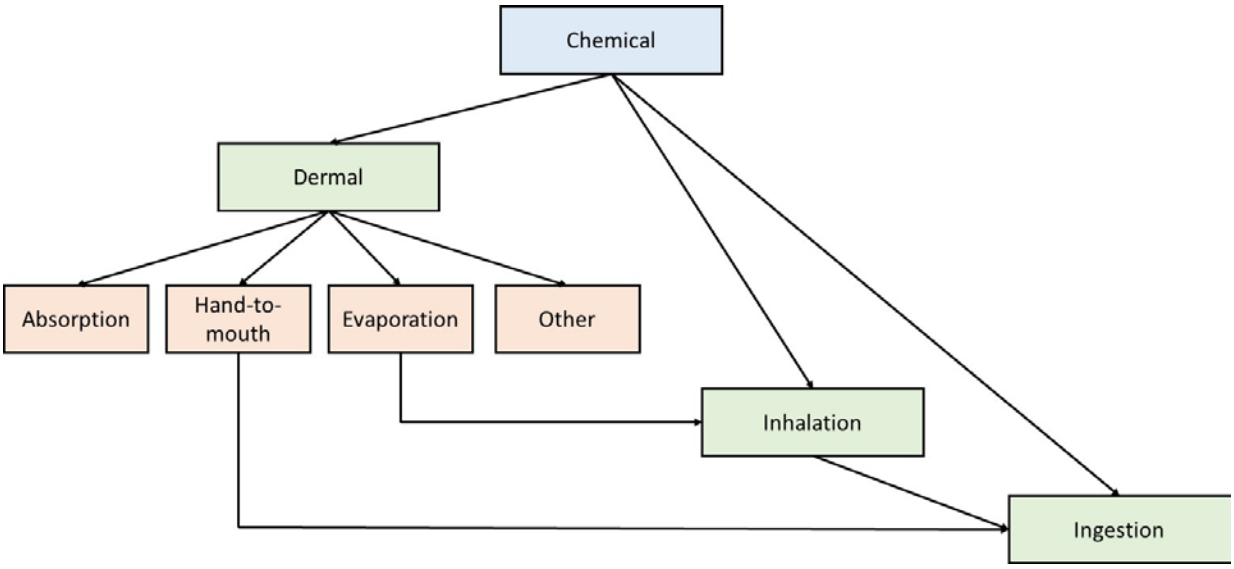

Figure 4. Direct exposure routes.

8.2 Direct dermal exposure

Direct dermal exposure occurs during both the active use and post-use phases. Given that many of the modeling concepts are the same in both active and post-use phases, this section first describes the general equations and assumptions applicable to both use phases, before applying these equations to each of the active and post-use phases.

8.2.1 General overview of equations and assumptions

This section provides the general equations for direct dermal exposure applicable to both active use and post-use phases. These equations are then tailored for active use and post-use in their respective sections.

To evaluate the competing removal processes for dermal exposure, the Direct Exposure model expands on the mass transfer equations of Ernstoff et al. (Ernstoff, Fantke et al. 2016) to include terms for hand-to-mouth transfer and other removal (e.g., rubbing off, handwashing, transfer to other surfaces). Each removal process is modeled as a first-order exponential decay with a specified rate constant. The sum of the processes is also a first-order decay, with a rate constant equal to the sum of the individual rate constants, as shown below:

$$k_{sk,lost} = k_{sk,abs} + k_{sk,evap} + k_{sk,oth} + k_{sk,hm} \quad (121)$$

where:

$k_{sk,lost}$ = rate constant for overall dermal loss [h^{-1}]
$k_{sk,abs}$ = rate constant for absorption from skin surface into stratum corneum [h^{-1}]
$k_{sk,evap}$ = rate constant for evaporation from skin surface to air [h^{-1}]
$k_{sk,oth}$ = rate constant for other removal from skin surface [h^{-1}]
$k_{sk,hm}$ = rate constant for hand-to-mouth transfer [h^{-1}]

Values for $k_{sk,abs}$, $k_{sk,evap}$, $k_{sk,oth}$, and $k_{sk,hm}$ are provided for each chemical by the "eval.dermal.rates" function (see Section 5.7.1). Briefly, the rate constants for absorption into the stratum corneum ($k_{sk,abs}$) and evaporation from the skin surface ($k_{sk,evap}$) are calculated using formulas from Ernstoff et al. (Ernstoff, Fantke et al. 2016). The hand-to-mouth transfer rates are calculated using results from a custom version of EPA's SHEDS-Multimedia model designed to predict soil and dust ingestion rates (Ozkaynak, Xue et al. 2011), assuming that the fractional rate per hour is one-half of the ratio found empirically in those model runs (hand-to-mouth exposure to hand exposure). We assume that adults have the same hand-to-mouth transfer rate as 16-20 year olds. The last of the dermal removal processes, referred to as "other removal", has been set to a point value of zero for the current version of S2D. This inactivates the "other removal" process, but the equations are still present in the code, allowing the user the ability to use a non-zero value if desired.

Each time a product is used, the mass of chemical remaining on the skin and the total mass of chemical lost due to the competing removal processes are given as:

$$M_{c,sk} = M_{c,sk,0} \times exp^{-k_{sk,lost} \times t} \quad (122)$$

$$M_{c,sk,lost} = M_{c,sk,0} - M_{c,sk} = M_{c,sk,0} \times (1 - exp^{-k_{sk,lost} \times t}) \quad (123)$$

where:

$M_{c,sk}$ = mass of chemical remaining on the skin [mg]
$M_{c,sk,lost}$ = total mass of chemical lost due to all competing removal processes [mg]
$M_{c,sk,0}$ = initial mass of chemical on the skin [mg]
$k_{sk,lost}$ = rate constant for overall dermal loss [h^{-1}]

t = duration of use [h]

The chemical mass lost due to each competing process i is calculated as:

$$M_{c,sk,i} = f_{sk,i} \times M_{c,sk,lost} \quad (124)$$

$$f_{sk,i} = \frac{k_{sk,i}}{k_{sk,lost}} = \frac{k_{sk,i}}{k_{sk,abs} + k_{sk,evap} + k_{sk,oth} + k_{sk,hm}} \quad (125)$$

where:

$M_{c,sk,i}$ = mass of chemical lost due to competing process i [mg]
$f_{sk,i}$ = fraction of total mass of chemical removed due to competing process i [-]
$M_{c,sk,lost}$ = total mass of chemical lost due to all competing removal processes [mg]
$k_{sk,lost}$ = rate constant for overall dermal loss [h^{-1}]
$k_{sk,i}$ = rate constant for competing process i [h^{-1}]
i = one of four competing removal processes (i.e., absorption (abs), evaporation (evap), other removal (oth), hand-to-mouth transfer (hm)) [-]

To account for products that are subject to wipe-off or rinse-off, the above equations are multiplied by the fraction of the skin corresponding to hands and to the body to determine three outputs listed below. If a PUC does not have a value for the fraction of skin that corresponds to hands, a value of 0.05 is used.

(i) Dermal exposure on the hands and body. This is defined as the mass of chemical on the hands and body prior to any removal processes and is given by:

$$M_{c,hands,0} = f_{sk,hands} \times M_{c,sk,0} \quad (126)$$

$$M_{c,body,0} = f_{sk,body} \times M_{c,sk,0} \quad (127)$$

where:

$M_{c,hands,0}$ = initial mass of chemical on the hands [mg]
$M_{c,body,0}$ = initial mass of chemical on the body [mg]
$M_{c,sk,0}$ = initial mass of chemical on the skin [mg]
$f_{sk,hands}$ = fraction of the skin corresponding to hands [-]
$f_{sk,body}$ = fraction of the skin corresponding to body [-]

(ii) Chemical mass loading on the hands and body prior to any removal processes. This is defined as the per area mass of chemical on the hands and body and is given by:

$$M_{c,hands,load} = \frac{M_{c,hands,0}}{A_{hands}} \quad (128)$$

$$M_{c,body,load} = \frac{M_{c,body,0}}{A_{body}} \quad (129)$$

where:

$M_{c,hands,load}$	=	chemical mass loading on the hands [mg]
$M_{c,body,load}$	=	chemical mass loading on the body [mg]
$M_{c,hands,0}$	=	initial mass of chemical on the hands [mg]
$M_{c,body,0}$	=	initial mass of chemical on the body [mg]
A_{hands}	=	amount of prime skin area for hands [mg]
A_{body}	=	amount of prime skin area for body [mg]

Prime skin area is defined above, and varies by adult and child depending on the PUC. Values of A_{hands} and A_{body} are calculated by assuming that 5% of prime skin area is hands and 95% of prime skin area is body. The estimated surface areas of exposed body parts (trunk, hands, face, genital area, etc.) that come into contact with each PUC are defined as model inputs.

(iii) Dermal absorption into the hands and body. This is defined as the mass of chemical absorbed from the skin surface into the stratum corneum and is given by the mass lost due to the absorption removal process, or:

$$M_{c,hands,abs} = f_{sk,hands} \times M_{c,sk,abs} = f_{sk,hands} \times f_{sk,abs} \times M_{c,sk,0} \times (1 - exp^{-k_{sk,lost} \times t}) \quad (130)$$

$$M_{c,body,abs} = f_{sk,body} \times M_{c,sk,abs} = f_{sk,body} \times f_{sk,abs} \times M_{c,sk,0} \times (1 - exp^{-k_{sk,lost} \times t}) \quad (131)$$

where:

$M_{c,hands,abs}$	=	mass of chemical absorbed into the stratum corneum on the hands [mg]
$M_{c,body,abs}$	=	mass of chemical absorbed into the stratum corneum on the body [mg]
$f_{sk,hands}$	=	fraction of skin area corresponding to hands [-]
$f_{sk,body}$	=	fraction of skin area corresponding to body [-]
$M_{c,sk,abs}$	=	mass of chemical lost due to absorption from skin surface into stratum corneum [mg]
$f_{sk,abs}$	=	fraction of total mass of chemical removed due to absorption from skin surface into stratum corneum [-]
$M_{c,sk,0}$	=	initial mass of chemical on the skin [mg]
$k_{sk,lost}$	=	rate constant for overall dermal loss [h^{-1}]
t	=	duration of use [h]

These three outputs are determined for the primary individual in each household and are calculated as the sum of contributions from active use and post-use exposure.

8.2.2 Active use

During active use, the duration is short enough that it is assumed only two competing removal processes occur: absorption into the stratum corneum and evaporation. Although the duration time for hands and body is the same, separate equations for hands and body are maintained to be consistent with the post-use phase.

Applying the equations above, the chemical mass absorbed into the skin during the active use phase is given by:

$$M_{c,hands,abs,use} = f_{sk,hands} \times \frac{k_{sk,abs}}{k_{sk,abs} + k_{sk,evap}} \times M_{c,skin,use,0} \times (1 - exp^{-(k_{sk,abs}+k_{sk,evap})\times t_{use}}) \quad (132)$$

$$M_{c,body,abs,use} = f_{sk,body} \times \frac{k_{sk,abs}}{k_{sk,abs} + k_{sk,evap}} \times M_{c,skin,use,0} \times (1 - exp^{-(k_{sk,abs}+k_{sk,evap})\times t_{use}}) \quad (133)$$

$$M_{c,dermal,abs,use} = M_{c,hands,abs,use} + M_{c,body,abs,use} \quad (134)$$

where:

$M_{c,hands,abs,use}$	=	mass of chemical absorbed into the skin via the hands during the active use phase [mg]
$M_{c,body,abs,use}$	=	mass of chemical absorbed into the skin via the body during the active use phase [mg]
$M_{c,dermal,abs,use}$	=	mass of chemical absorbed into the skin during the active use phase [mg]
$M_{c,skin,use,0}$	=	initial mass of chemical on the skin during active use [mg]
t_{use}	=	duration of active use [h]
$f_{sk,hands}$	=	fraction of skin area corresponding to hands [-]
$f_{sk,body}$	=	fraction of skin area corresponding to body [-]
$k_{sk,abs}$	=	rate constant for absorption from skin surface into stratum corneum [h^{-1}]
$k_{sk,evap}$	=	rate constant for evaporation from skin surface to air [h^{-1}]
k_{oth}	=	rate constant for other removal from skin surface [h^{-1}]
k_{hm}	=	rate constant for hand-to-mouth transfer [h^{-1}]

The initial mass of chemical on the skin during active use, $M_{c,skin,use,0}$, is assumed to be the average mass during the active use phase (i.e., sum of the chemical mass at the beginning and end of the active use phase, divided by two).

Similarly, the mass of chemical released to the air through evaporation from the hands and body can be calculated. These equations are provided in the inhalation exposure section.

8.2.3 Post-use

For post-use dermal exposure, it is assumed that the chemical remains present on the body for eight hours, after which it disappears (by implicit washing or showering). Based on this assumption, the residence time that the chemical remains on hands is estimated as:

$$t_{post,h} = \frac{t_{post,b}}{hw} = \frac{8}{hw} \quad (135)$$

where:

$t_{post,h}$	=	post-use residence time on hands [h]
$t_{post,b}$	=	post-use residence time on body [h]
hw	=	number of handwashing events per day, varies by person [-]

For the post-use phase, all four competing processes are assumed to occur for hands; however, only three of the processes are considered to occur for the body (i.e., there is no chemical transfer from the body to the mouth).

Applying equations above to the post-use phase, the mass of chemical absorbed into the skin during the post-use phase is given by:

$$M_{c,hands,abs,post} = f_{sk,hands} \times \frac{k_{sk,abs}}{k_{sk,abs} + k_{sk,evap} + k_{oth} + k_{hm}} \times M_{c,skin,post,0} \times (1 - exp^{-(k_{sk,abs}+k_{sk,evap}+k_{oth}+k_{hm})\times t_{post,h}}) \quad (136)$$

$$M_{c,body,abs,post} = f_{sk,body} \times \frac{k_{sk,abs}}{k_{sk,abs} + k_{sk,evap} + k_{oth}} \times M_{c,skin,post,0} \times (1 - exp^{-(k_{sk,abs}+k_{sk,evap}+k_{oth})\times t_{post,b}}) \quad (137)$$

$$M_{c,dermal,abs,post} = M_{c,hands,abs,post} + M_{c,body,abs,post} \quad (138)$$

where:

$M_{c,hands,abs,post}$	=	mass of chemical absorbed into the skin via the hands during the post-use phase [mg]
$M_{c,body,abs,post}$	=	mass of chemical absorbed into the skin via the body during the post-use phase [mg]
$M_{c,dermal,abs,post}$	=	mass of chemical absorbed into the skin during the post-use phase [mg]
$M_{c,skin,post,0}$	=	initial mass of chemical on the skin during post-use [mg]
$t_{post,h}$	=	post-use residence time on hands [h]
$t_{post,b}$	=	post-use residence time on body [h]
$f_{sk,hands}$	=	fraction of skin area corresponding to hands [-]

$f_{sk,body}$ = fraction of skin area corresponding to body [-]
$k_{sk,abs}$ = rate constant for absorption from skin surface into stratum corneum [h^{-1}]
$k_{sk,evap}$ = rate constant for evaporation from skin surface to air [h^{-1}]
k_{oth} = rate constant for other removal from skin surface [h^{-1}]
k_{hm} = rate constant for hand-to-mouth transfer [h^{-1}]

The initial mass of chemical on the skin during the post-use phase, $M_{c,skin,post,0}$, is assumed to be the mass at the end of the post-use phase.

Similar equations can be written for the loss of chemical mass from the hands and body to the other competing removal processes during the post-use phase. These equations are found in the inhalation and ingestion exposure sections (Sections 8.3 and 8.4) for loss by evaporation and loss by hand-to-mouth transfer, respectively.

8.2.4 Output metrics

Each time a product is used, the overall dermal exposure, maximum chemical mass loading, and dermal absorption is calculated by summing together the contributions from the active use and post-use phases.

$$M_{c,dermal,0} = M_{c,hands,use,0} + M_{c,body,use,0} + M_{c,hands,post,0} + M_{c,body,post,0} \quad (139)$$

$$M_{c,dermal,maxload} = \max(M_{c,hands,load,use}, M_{c,body,load,use}, M_{c,hands,load,post}, M_{c,body,load,post}) \quad (140)$$

$$M_{c,dermal,abs} = M_{c,hands,abs,use} + M_{c,body,abs,use} + M_{c,hands,abs,post} + M_{c,body,abs,post} \quad (141)$$

where:

$M_{c,dermal,0}$ = overall dermal exposure to product [mg]
$M_{c,dermal,maxload}$ = maximum chemical mass loading [mg]
$M_{c,dermal,abs}$ = mass of chemical absorbed into skin [mg]
$M_{c,hands,use,0}$ = initial mass of chemical on the hands during active use [mg]
$M_{c,body,use,0}$ = initial mass of chemical on the body during active use [mg]
$M_{c,hands,post,0}$ = initial mass of chemical on the hands during post-use [mg]
$M_{c,body,post,0}$ = initial mass of chemical on the body during post-use [mg]
$M_{c,hands,load,use}$ = chemical mass loading on the hands during active use [mg]
$M_{c,body,load,use}$ = chemical mass loading on the body during active use [mg]
$M_{c,hands,load,post}$ = chemical mass loading on the hands during post-use [mg]
$M_{c,body,load,post}$ = chemical mass loading on the body during post-use [mg]
$M_{c,hands,abs,use}$ = mass of chemical absorbed into the stratum corneum on the hands during active use [mg]
$M_{c,body,abs,use}$ = mass of chemical absorbed into the stratum corneum on the body during active use [mg]

$M_{c,hands,abs,post}$ = mass of chemical absorbed into the stratum corneum on the hands during post-use [mg]

$M_{c,body,abs,post}$ = mass of chemical absorbed into the stratum corneum on the body during post-use [mg]

To calculate the daily output metrics, the diary events from the product-use scheduler are used to identify when products are used. Hand and body exposure and absorption contributions from each instance of product use over the course of the day are summed together (or the max is identified) to get the daily dermal exposure (dir.derm.exp, Table 2), daily maximum chemical mass loading (dir.derm.max), and daily dermal absorption (dir.derm.abs). Once a chemical is dermally absorbed, it is no longer tracked by the S2D module after it enters the human body.

8.3 Direct inhalation exposure

Direct inhalation exposure occurs during both the active use and post-use phases. Given that many of the modeling concepts are the same in both active use and post-use phases, this section first describes the general equations and assumptions applicable to both active use and post-use phases, before applying these equations to each of the active and post-use phases.

8.3.1 General overview of equations and assumptions

This section provides the general equations for direct inhalation exposure applicable to both active use and post-use phases. These equations are then tailored for active use and post-use in their respective sections.

The basic S2D code uses the daily average air concentration to which a person is exposed as a proxy for inhalation exposure. In this version of the model, only indoor air exposure is considered (i.e., inhalation exposure due to outdoor product use or evaporation from skin to outdoor air is not considered).

During the active use and post-use phases, the only chemical transfer process that is assumed to occur is evaporation from the skin surface into air. As a result, the mass of chemical in the air can be calculated as:

$$M_{c,air} = M_{c,air,0} + M_{c,hands,evap} + M_{c,body,evap} \quad (142)$$

where:

$M_{c,air}$ = mass of chemical in the air [mg]

$M_{c,air,0}$ = mass of chemical placed in the air by product use [mg]

$M_{c,hands,evap}$ = mass of chemical transferred into the air due to evaporation from the hands [mg]

$M_{c,body,evap}$ = mass of chemical transferred into the air due to evaporation from the body [mg]

The mass of chemical transferred into the air from the hands and body were previously defined in above equations.

The chemical that evaporates from the skin is assumed to enter a personal cloud, defined as the immediate space surrounding the person, and may be inhaled. The concentration of the chemical in air that a person is exposed to is calculated by balancing the chemical inflow and outflow for the cloud. The inflow is chemical mass per unit time [mg/hr], where the time represents either the duration of product use, or the duration that chemical resides on the skin post-use.

$$inflow = \frac{mass\ evaporating}{duration} = \frac{M_{c,air}}{duration}$$

$$outflow = C_{c,air} \times V_{cloud} \times aer_{cloud} \quad (143)$$

Hence:

$$C_{c,air} = \frac{M_{c,air}}{V_{cloud} \times aer_{cloud} \times duration}$$

where:

$inflow$	=	chemical inflow into the personal cloud [mg/hr]
$M_{c,air}$	=	mass of chemical in the air [mg]
$duration$	=	duration of product use or duration that chemical resides on the skin post-use [hr]
$outflow$	=	chemical flow out of the personal cloud [mg/hr]
$C_{c,air}$	=	concentration of chemical in the air (in the personal cloud) [mg/m^3]
V_{cloud}	=	personal cloud volume [m^3]
aer_{cloud}	=	air exchange rate between the personal cloud and the house [hr^{-1}]

As the duration of both the active use and post-use phases are defined in the S2D module to be less than one day, a daily inhalation exposure can be calculated by adjusting/scaling the air concentration to one day as follows:

$$C_{c,air,dailyexp} = C_{c,air} \times \frac{t}{24} \quad (144)$$

where:

$C_{c,air,dailyexp}$	=	daily inhalation exposure [mg/m^3]
t	=	exposure duration [h]

The mass of air inhaled is calculated based on the basal or baseline breathing ventilation rate (i.e., when a person is lying down) and a metabolic energy multiplier (met) that accounts for whether a person is awake or asleep.

$$M_{c,inhal} = C_{c,dailyexp} \times r_{vent} \times met \quad (145)$$

where:

$M_{c,inhal}$	=	mass of air inhaled over one day [mg]
r_{vent}	=	basal ventilation rate [m^3/day]

met = metabolic energy multiplier [-]

In the current version of the module, baseline breathing ventilation rates based on age and sex were obtained from the APEX model (U.S. EPA 2012, U.S. EPA 2012). The equations to calculate the ventilation rates may also be integrated into the RPGen module if desired in the future. While different diary activities will have different met values, the S2D code does consider individual activities and instead uses an average met value for all activities associated with a PUC. The met values used in this code were obtained from the PUC_MET.csv input file, where they are described as "Mean METS from APEX" and are point values representing the mean value for each activity.

Once a chemical is inhaled, the mass absorbed into the blood is calculated as given by:

$$M_{c,inhal,abs} = M_{c,inhal} \times f_{inhal,abs} \quad (146)$$

where:

$M_{c,inhal,abs}$ = mass of chemical absorbed into the blood through inhalation [mg]
$f_{inhal,abs}$ = mass fraction absorbed into the blood [-]

The mass fraction absorbed into the blood was set to 16% in the S2D code (as used in SHEDS-HT (Isaacs, Glen et al. 2014).

Similar to direct dermal exposure, contributions to inhalation exposure due to the active use and post-use phases must first be calculated before summing them together over all product uses (or finding the max) to arrive at overall daily inhalation exposure metrics (dir.inhal.exp, dir.inhal.max, dir.inhal.mass, and dir.inhal.abs in Table 2).

8.3.2 Active use

During active use, the mass of chemical in the air ($M_{c,air,use}$) is defined as:

$$M_{c,air,use} = M_{c,air,use,0} + M_{c,hands,evap,use} + M_{c,body,evap,use} \quad (147)$$

where:

$M_{c,air,use}$ = mass of chemical in the air during active use [mg]
$M_{c,air,use,0}$ = initial mass of chemical in the air during active use [mg]
$M_{c,hands,evap,use}$ = mass transferred into the air due to evaporation from the hands during active use [mg]
$M_{c,body,evap,use}$ = mass transferred into the air due to evaporation from the body during active use [mg]

Following equations above, the mass transferred into the air from the hands and the body is given by:

$$M_{c,hands,evap,use} =$$

$$f_{sk,hands} \times \frac{k_{sk,evap}}{k_{sk,abs}+ k_{sk,evap}} \times M_{c,skin,use,0} \times (1 - exp^{-(k_{sk,abs}+k_{sk,evap})\times t_{use}}) \quad (148)$$

$$M_{c,body,evap,use} = f_{sk,body} \times \frac{k_{sk,evap}}{k_{sk,abs}+ k_{sk,evap}} \times M_{c,skin,use,0} \times (1 - exp^{-(k_{sk,abs}+k_{sk,evap})\times t_{use}}) \quad (149)$$

where:

$M_{c,hands,evap,use}$	=	mass transferred into the air due to evaporation from the hands during active use [mg]
$M_{c,body,evap,use}$	=	mass transferred into the air due to evaporation from the body during active use [mg]
$f_{sk,hands}$	=	fraction of skin corresponding to hands [-]
$f_{sk,body}$	=	fraction of skin corresponding to body [-]
$k_{sk,evap}$	=	rate constant for evaporation from skin surface to air [h^{-1}]
$k_{sk,abs}$	=	rate constant for absorption from skin surface into stratum corneum [h^{-1}]
$M_{c,skin,use,0}$	=	initial mass of chemical on the skin during active use [mg]
t_{use}	=	duration of active use [h]

During active use, the product handling time is the time over which the evaporated chemical mass is released. The equation for the chemical concentration in the personal cloud and the contribution to the daily average exposure are:

$$C_{c,air,use} = \frac{M_{c,air,use}}{V_{cloud} \times aer_{cloud} \times t_{use}} \quad (150)$$

$$C_{c,air,dailyexp,use} = C_{c,air,use} \times \frac{t_{use}}{24} \quad (151)$$

where:

$C_{c,air,use}$	=	concentration of chemical in the air during active use [mg/m^3]
$C_{c,air,dailyexp,use}$	=	daily inhalation exposure (from this source) during active use [mg/m^3]
$M_{c,air,use}$	=	mass of chemical in the air during active use [mg]
V_{cloud}	=	personal cloud volume during active use [m^3]
aer_{cloud}	=	air exchange rate between the personal cloud and the house [hr^{-1}]
t_{use}	=	duration of active product use [h]

The mass inhaled and the mass absorbed during the active use phase are then given by:

$$M_{c,inhal,use} = C_{c,air,use} \times \frac{t_{use}}{24} \times r_{vent} \times met \quad (152)$$

$$M_{c,inhal,abs,use} = 0.16 \times M_{c,inhal,use} \quad (153)$$

where:

$M_{c,inhal,use}$	=	mass of chemical inhaled during active use [mg]

$M_{c,inhal,abs,use}$ = mass of chemical absorbed into the blood through inhalation during active use [mg]
$C_{c,air,use}$ = concentration of chemical in the air during active use [mg/m^3]
t_{use} = duration of active product use [h]
r_{vent} = basal ventilation rate [m^3/day]
met = metabolic energy multiplier [-]

Note that for products in spray form, during active use, it is assumed that only 25% of the mass inhaled remains in the inhalation exposure route, with the remaining 75% allocated to the ingestion exposure route. As a result, the mass inhaled and the mass absorbed during the active use phase for spray products is given by:

$$M_{c,inhal,use,sprays} = \left(C_{c,air,use} \times \frac{t_{use}}{24} \times r_{vent} \times met\right) \times 0.25 \quad (154)$$

$$M_{c,inhal,abs,use,sprays} = 0.16 \times M_{c,inhal,use,sprays} \quad (155)$$

where:
$M_{c,inhal,use,sprays}$ = mass of chemical inhaled during active use for spray PUCs [mg]
$M_{c,inhal,abs,use,sprays}$ = mass of chemical absorbed into the blood through inhalation during active use of spray PUCs [mg]

8.3.3 Post-use

During post-use, the mass of chemical transferred into the air is defined as:

$$M_{c,air,post} = M_{c,hands,evap,post} + M_{c,body,evap,post} \quad (156)$$

where:
$M_{c,air,post}$ = mass of chemical in the air during post-use [mg]
$M_{c,hands,evap,post}$ = mass transferred into the air due to evaporation from the hands during post-use [mg]
$M_{c,body,evap,post}$ = mass transferred into the air due to evaporation from the body during post-use [mg]

It is assumed that no mass is present in the air at the beginning of the post-use phase (i.e., all chemical mass that a person is exposed to during the post-use phase is due to evaporation from the skin). Applying above equations, the mass of chemical evaporated from the hands and the body is given by:

$$M_{c,hands,evap,post} = f_{sk,hands} \times \frac{k_{sk,evap}}{k_{sk,abs} + k_{sk,evap} + k_{oth} + k_{hm}} \times M_{c,skin,0} \times \left(1 - exp^{-(k_{sk,abs}+k_{sk,evap}+k_{oth}+k_{hm})\times t_{post,h}}\right) \quad (157)$$

$$M_{c,body,evap,post} = f_{sk,body} \times \frac{k_{sk,evap}}{k_{sk,abs} + k_{sk,evap} + k_{sk,oth}} \times M_{c,skin,use,0} \times (1 - exp^{-(k_{sk,abs}+k_{sk,evap}+k_{sk,oth})\times t_{use}}) \quad (158)$$

S2D currently assumes a post-use duration of 8 hours. To account for evaporation of chemical from the skin during the post-use phase, the average inflow to the personal cloud is matched to the average outflow. The average inflow to the personal cloud is the mass lost from the skin to air, divided by the time (8 hours). The average outflow is the chemical mass in the cloud multiplied by the air exchange rate between the cloud and the surrounding air. The chemical mass in the cloud equals the air concentration multiplied by the cloud volume.

$$inflow = \frac{mass\ evaporating}{duration} = \frac{M_{c,air}}{8}$$

$$outflow = C_{c,air} \times V_{cloud} \times aer_{cloud} \quad (159)$$

Hence:

$$C_{c,air} = \frac{M_{c,air}}{V_{cloud} \times aer_{cloud} \times 8}$$

where:

$inflow$	=	chemical inflow into the personal cloud [mg/hr]
$M_{c,air}$	=	mass of chemical in the air [mg]
$outflow$	=	chemical out of the personal cloud [mg/hr]
$C_{c,air}$	=	concentration of chemical in the air (in the personal cloud) [mg/m^3]
V_{cloud}	=	personal cloud volume [m^3]
aer_{cloud}	=	air exchange rate between the personal cloud and the house [hr^{-1}]

8.3.4 Output metrics

Each time a product is used, the maximum air concentration, inhalation exposure (which is the air concentration adjusted to be a daily average), mass of chemical inhaled, and mass of chemical absorbed into the blood can be calculated by summing up the contributions from the active use and post-use phases.

$$C_{c,inhal,maxconc} = \max(C_{c,air,use}, C_{c,air,post}, C_{c,inhal,exp}) \quad (160)$$

$$C_{c,inhal,exp} = C_{c,air,exp,use} + C_{c,air,exp,post} \quad (161)$$

$$M_{c,inhal} = M_{c,inhal,use} + M_{c,inhal,post} \quad (162)$$

$$M_{c,inhal,abs} = M_{c,inhal,abs,use} + M_{c,inhal,abs,post} \quad (163)$$

where:

$C_{c,inhal,maxconc}$	=	maximum air concentration [mg/m^3]
$C_{c,inhal,exp}$	=	daily inhalation exposure [mg/m^3]
$M_{c,inhal}$	=	mass of chemical inhaled [mg]
$M_{c,inhal,abs}$	=	mass of chemical absorbed into the blood due to inhalation [mg]

The daily values of the four inhalation metrics (dir.inhal.exp, dir.inhal.max, dir.inhal.mass, and dir.inhal.abs in Table 2) are then calculated by summing together the contributions (or finding the max) from each product use.

8.4 Direct ingestion exposure

Both direct ingestion, which may occur for products such as toothpaste, mouthwash, and similar products, and hand-to-mouth ingestion are modeled using mass partitioning into the gut compartment. Note that the current version of the S2D module does not model food or water consumption.

As direct ingestion only occurs during active use and hand-to-mouth transfer only occurs in post-use, the equations used to calculate the mass ingested in each of these use phases are presented below in their respective sections.

8.4.1 General overview of equations and assumptions

For both active use and post-use phases, once a chemical is ingested, the mass absorbed into the gut is calculated as:

$$M_{c,ingest,abs} = M_{c,ingest} \times f_{ingest,abs} \quad (164)$$

where:

$M_{c,ingest,abs}$	=	mass of chemical absorbed into the gut [mg]
$M_{c,ingest}$	=	mass of chemical ingested [mg]
$f_{ingest,abs}$	=	mass fraction absorbed into the gut [-]

The mass fraction absorbed into the gut varies for each PUC and are provided as model inputs.

8.4.2 Active use

For oral products such as toothpaste, the mass ingested is calculated based on the initial transfer into the gut that a chemical undergoes at the start of product use:

$$M_{c,ingest,use} = M_c \times f_{gi} \quad (165)$$

where:

$M_{c,ingest,use}$	=	mass of chemical ingested during active use [mg]
M_c	=	initial mass of chemical in the product [mg]
f_{gi}	=	mass fraction that transfers into the gut [-]

As previously mentioned, for spray PUCs, it is assumed that in addition to the initial partitioning into the gut, 75% of the mass inhaled is assumed to be ingested during active use. The resulting mass of chemical ingested and absorbed into the gut during active use, for spray PUCs, is then given by:

$$M_{c,ingest,use,sprays} = (M_c \times f_{gi}) + 0.75 \times \left(\frac{M_{c,air,use}}{0.5 \times t_{use}} \times \frac{t_{use}}{24} \times r_{vent} \times met\right) \quad (166)$$

$$M_{c,ingest,abs,use,sprays} = M_{c,ingest,use,sprays} \times f_{ingest,abs} \quad (167)$$

where:

$M_{c,ingest,use,sprays}$	=	mass of chemical ingested during active use for spray PUCs [mg]
$M_{c,ingest,abs,use,sprays}$	=	mass of chemical absorbed during active use for spray PUCs [mg]

8.4.3 Post use

Hand-to-mouth ingestion occurs only during post use when a person is not careful and assumes that their hands are clean. Applying equations derived in the Dermal Exposure section for hand-to-mouth transfer, the mass of chemical ingested via this exposure route is given by:

$$M_{c,ingest,post} = M_{c,hands,hm,post} \quad (168)$$

$$M_{c,hands,hm,post} = f_{sk,hands} \times \frac{k_{hm}}{k_{sk,abs} + k_{sk,evap} + k_{oth} + k_{hm}} \times M_{c,skin,0} \times (1 - exp^{-(k_{sk,abs}+k_{sk,evap}+k_{oth}+k_{hm})\times t_{post,h}}) \quad (169)$$

where:

$M_{c,ingest,post}$	=	mass of chemical ingested during post-use [mg]
$M_{c,hands,hm,post}$	=	mass of chemical transferred from hands to mouth during post-use [mg]

The mass absorbed into the gut is then:

$$M_{c,ingest,abs,post} = M_{c,ingest,post} \times f_{ingest,abs} \quad (170)$$

where:

$M_{c,ingest,abs,post}$	=	mass of chemical absorbed during post-use [mg]

$f_{ingest,abs}$ = mass fraction absorbed into the gut [-]

8.4.4 Output metrics

For each product use, two ingestion output metrics can be calculated by summing up the contributions from the active use and post-use phases: ingestion exposure (which corresponds to the mass of chemical ingested) and ingestion absorption (which is equal to the mass of chemical ingested that is absorbed into the gut).

$$M_{c,ingest,exp} = M_{c,ingest,use} + M_{c,ingest,post} \quad (171)$$

$$M_{c,ingest,abs} = M_{c,ingest,abs,use} + M_{c,ingest,abs,post} \quad (172)$$

where:

$M_{c,ingest,exp}$ = ingestion exposure, equal to the mass of chemical ingested [mg]

$M_{c,ingest,abs}$ = ingestion absorption, equal to the mass of chemical absorbed into the gut [mg]

Daily output metrics (dir.ingest.exp and dir.ingest.abs in Table 2) are then calculated by summing up the $M_{c,ingest,exp}$ and $M_{c,ingest,abs}$ contributions from each instance of product use over the day.

9. Indirect Exposure function: eval.indirect()

The Indirect Exposure function calculates route-specific dermal, inhalation, and ingestion chemical exposures for the primary individual in each household due to indirect sources. Note that in this usage, "primary" refers to the individual chosen by RPGen to have their exposure fully assessed, and is not an indicator of age or status. Sources of indirect exposure occur after product use has ceased and include contributions from the activities of all members of the household to communal air and surface loadings through their personal product use (which are assessed by the Fugacity function), and delayed exposure from the primary individual's earlier activities. The approach used to calculate indirect exposure are similar to those used to calculate direct exposure (see Section 8); however, the calculations are slightly different as the Indirect Exposure function first computes an hourly time series which is then used to arrive at daily indirect exposure metrics. This differs from direct exposure, which has no hourly calculations and goes directly from exposure per product use to exposure per day. The exposure routes and exposure periods are described in the following section.

Inputs

d	all the diary activity events of the primary individual in the household
fug.hour	hourly mass of each chemical in the air and surface compartments after the fugacity calculations are complete
dermal.rates	information on the rate constants for the four competing chemical removal processes from the skin surface: absorption into the stratum corneum,

	evaporation into the air, hand-to-mouth transfer, and other removal (e.g., rubbing off, handwashing, transfer to other surfaces)
hp	specific house properties
nc	number of chemicals being modeled in the current model run
prime	demographic information on the primary individual and exposure factors such as basal ventilation rate, skin surface area, hand washing, and hand to mouth transfer rates
fug.cvars	chemical properties of each chemical
chem.list	all the chemicals

Outputs

indirect	daily indirect exposure metrics (Table 2) including the dermal exposure (ind.derm.exp, mg), dermal maximum loading (ind.derm.max, mg/cm^2), dermal absorbed dose (ind.derm.abs, mg), inhalation exposure (ind.inhal.exp, mg/m^3), inhaled mass (ind.inhal.mass, mg), maximum air concentration (ind.inhal.max, mg/m^3), inhaled mass of chemical absorbed (ind.inhal.abs, mg), ingested chemical mass (ind.ingest.exp, mg), ingested chemical mass absorbed (ind.ingest.abs, mg) for each chemical

9.1 Overview of exposure routes and exposure periods

Similar to the Direct Exposure function, the Indirect Exposure function in S2D considers three exposure routes (dermal, inhalation, and ingestion). As exposure to indirect sources is first calculated using hourly exposure values, which are then used to obtain daily exposure values, each hour is evaluated to determine the exposure period(s) that an activity occurs in. Three exposure periods are considered in S2D, corresponding to periods when the primary person is asleep, awake at home, or away from home.

For each hour of the 364-day year, the activities in the household diaries output from the Product Use Scheduler are examined to determine the number of minutes in each of the three exposure periods. It is assumed that for weekdays, lunch occurs away from home. The number of minutes in each hour corresponding to asleep, awake at home, and away from home are matched up with the hourly time-series data for air and surface concentrations produced by the Fugacity function. For any hour with partial time awake at home or with time spent sleeping, only the fraction of hour available for indirect exposure is considered. For the purposes of determining outputs such as the maximum instantaneous air concentration and dermal loading, partial hours are not considered, because for the direct exposure, the maximum values are instantaneous since often they last only the duration of product use, which may be as short as one minute.

All these factors are then applied to the hourly time series of adjusted air and surface concentrations. Note that here "adjusted" means that hours that do not qualify for the daily maximum air concentration or daily maximum dermal loading are removed from consideration by setting their values to zero. These adjusted time series are folded into matrix form (24 hours x 364 days), and the daily values are computed.

Depending on the period of exposure, indirect dermal, inhalation, and ingestion exposure will occur as follows:

Asleep at home. Each hour spent sleeping at home leads to inhalation exposure for that hour.

Awake at home. Each hour spent awake at home leads to inhalation exposure for that hour. Time spent awake at home also leads to dermal exposure by contact with chemical-containing surfaces, and for persons with significant hand-to-mouth contact, there will also be indirect ingestion exposure.

Away from home. Each hour spent away from home results in no indirect exposure.

9.2 Indirect dermal exposure

9.2.1 General overview

Indirect dermal exposure occurs as a result of contact with chemical-containing surfaces. Similar to direct dermal exposure, the same four competing removal processes are considered and modeled as a first-order exponential decay with a specified rate constant. Unlike direct dermal exposure, there is no variable contact duration when assessing indirect exposure (as opposed to direct dermal exposure when active use and post-use durations are considered). Instead, the duration is always assumed to be eight hours divided by the number of hand washes per day. Hence, there is always a given fraction of indirect dermal exposure that is absorbed for each chemical, and the same fraction applies to all hours of the year which have any indirect contact.

Indirect exposure is evaluated hourly. For dermal exposure, the chemical may be assumed to reside on the hands for more than one hour. As seen below, the time "t" in the dermal removal equation is set to t=8/hw, which exceeds one hour when hw<8 (handwashes per day). This does not affect the calculation for other hours, because the fate of the chemical picked up by the hands is resolved on the current hour. In effect, the amount that would eventually be removed by each process (as determined by the equations below) is immediately removed, so the next hour starts with effectively no dermal loading.

The three outputs, namely dermal exposure, maximum chemical mass loading, and dermal absorption, can be calculated as described below.

(i) Dermal exposure on the hands. This is defined as the mass of chemical on the hands due to transfer from chemical-containing surfaces, prior to any removal processes, and is given by the equations below. The S2D code currently assumes that only the hands contact such surfaces, although it would be possible to include a body exposure term as well in future

versions of the code, and uses a transfer coefficient approach to determine the amount of chemical transferred from surfaces to skin. The transfer coefficient for hands is assumed to be 300 cm^2/hr and the fraction of skin area corresponding to hands is assumed to be 5%. In addition, similar to SHEDS-HT (Isaacs, Glen et al. 2014), S2D also uses a variable, referred to as fraction of the chemical loading available for transfer, to reflect the fact that in some cases, the chemical is not easily extracted from the objects to which it is bound. Fraction of the chemical loading available for transfer was set constant at 0.5, the same value used in SHEDS-HT.

$$M_{c,hands,0} = C_{sur} \times tc \times f_{avail} \times f_{awake} \quad (173)$$

$$C_{sur} = \frac{C_{sur,fug}}{A_{sur} \times 10000} \quad (174)$$

$$f_{awake} = \frac{t_{awake}}{60}$$

where:

$M_{c,hands,0}$	=	initial mass (exposure) of chemical on the hands due to indirect exposure picked up on the current hour [mg]
C_{sur}	=	chemical concentration on surfaces [mg/cm^2]
$C_{sur,fug}$	=	surface concentrations from the fugacity function [mg/m^3]
A_{sur}	=	surface area of house [m^2]
tc	=	transfer coefficient for hands [cm^2/h], set to 300
f_{avail}	=	fraction of the chemical loading available for transfer [-], set to 0.5
f_{awake}	=	fraction of the hour spent awake at home [-]
t_{awake}	=	minutes in an hour spent awake at home [min]

(ii) Chemical mass loading on the hands prior to any removal processes. This is defined using the same equation as used for direct exposure:

$$M_{c,hands,load} = \frac{M_{c,hands,0}}{A_{hands}} \quad (175)$$

where:

$M_{c,hands,load}$	=	chemical mass loading on the hands [mg]
A_{hands}	=	amount of prime skin area for hands [m^2]

(iii) Dermal absorption into the hands. This is defined as the mass of chemical absorbed from the skin surface into the stratum corneum and uses the same equations defined in the Direct Exposure function for the mass lost due to the absorption removal process:

$$M_{c,hands,abs} = M_{c,hands,0} \times f_{sk,abs} \times (1 - exp^{-k_{sk,lost} \times t}) \quad (176)$$

$$f_{sk,abs} = \frac{k_{sk,abs}}{k_{sk,lost}} = \frac{k_{sk,abs}}{k_{sk,abs} + k_{sk,evap} + k_{sk,oth} + k_{sk,hm}} \quad (177)$$

$$t = \frac{8}{hw} \quad (178)$$

where:

$M_{c,hands,abs}$	=	mass of chemical absorbed into the stratum corneum on the hands [mg]
$f_{sk,abs}$	=	fraction of total mass of chemical removed due to absorption into skin [-]
$k_{sk,lost}$	=	rate constant for overall dermal loss [h^{-1}]
$k_{sk,abs}$	=	rate constant for absorption from skin surface into stratum corneum [h^{-1}]
$k_{sk,evap}$	=	rate constant for evaporation from skin surface to air [h^{-1}]
$k_{sk,oth}$	=	rate constant for other removal from skin surface [h^{-1}]
$k_{sk,hm}$	=	rate constant for hand-to-mouth transfer [h^{-1}]
t	=	duration of indirect exposure [h]
hw	=	number of handwashing events per day, varies by person [-]

9.2.2 Output metrics

For each hour, the above three outputs are determined for the primary individual in each household. To calculate daily (Table 2) dermal exposure (ind.derm.exp), daily maximum chemical mass loading (ind.derm.max), and daily dermal absorption (ind.derm.abs), the 24 hourly values are either summed together or the maximum hourly value is selected, as shown below. For simplicity, these post-contact exposures are assigned to the same hour as the initial contact.

$$M_{c,dermal,0,daily} = \sum_{i=1}^{24} M_{c,hands,0,i} \quad (179)$$

$$M_{c,dermal,maxload,daily} = \max(hourly\ M_{c,hands,load}) \quad (180)$$

$$M_{c,dermal,abs,daily} = \sum_{i=1}^{24} M_{c,hands,abs,i} \quad (181)$$

where:

$M_{c,dermal,0}$	=	overall dermal exposure to product [mg]
$M_{c,dermal,maxload}$	=	maximum chemical mass loading [mg]
$M_{c,dermal,abs}$	=	dermal absorption into skin [-]

9.3 Indirect ingestion exposure

9.3.1 General overview

For persons with significant hand-to-mouth contact, there will be indirect ingestion exposure resulting from dermal contact with surfaces. This will be proportional to the indirect dermal exposure, with the ratio depending on age. As the duration of indirect contact is assumed to be eight hours divided by the

number of hand washes per day, and therefore a given fraction of dermal exposure is ingested for every chemical, the same fraction applies to all hours of the year which have any indirect contact.

Similar to post-use direct exposure, the indirect ingestion exposure resulting from hand-to-mouth exposure is given by:

$$M_{c,ingest} = M_{c,hands,0} \times f_{sk,hm} \times (1 - exp^{-k_{sk,lost} \times t}) \quad (182)$$

$$f_{sk,hm} = \frac{k_{sk,hm}}{k_{sk,lost}} = \frac{k_{sk,hm}}{k_{sk,abs} + k_{sk,evap} + k_{sk,oth} + k_{sk,hm}} \quad (183)$$

$$t = \frac{8}{hw} \quad (184)$$

where:

$M_{c,ingest}$	=	mass of chemical ingested [mg]
$M_{c,hands,0}$	=	initial mass of chemical on the hands [mg]
$f_{sk,hm}$	=	fraction of overall dermal loss due to hand-to-mouth transfer [-]
$k_{sk,lost}$	=	rate constant for overall dermal loss [h^{-1}]
$k_{sk,hm}$	=	rate constant for hand-to-mouth transfer [h^{-1}]
$k_{sk,abs}$	=	rate constant for absorption from skin surface into stratum corneum [h^{-1}]
$k_{sk,evap}$	=	rate constant for evaporation from skin surface to air [h^{-1}]
$k_{sk,oth}$	=	rate constant for other removal from skin surface [h^{-1}]
t	=	duration of indirect contact [h]
hw	=	number of handwashing events per day, varies by person [-]

The mass absorbed into the gut is then:

$$M_{c,ingest,abs} = M_{c,ingest} \times f_{ingest,abs} \quad (185)$$

where:

$M_{c,ingest,abs,post}$	=	mass of chemical absorbed during post-use [mg]
$f_{ingest,abs}$	=	mass fraction absorbed into the gut [-]

9.3.2 Output metrics

To calculate daily ingestion exposure and absorption (Table 2), the 24 hourly ingestion values are summed together as shown below. For simplicity, these post-contact exposures are assigned to the same hour as the initial contact.

$$ind.ingest.exp = \sum_{i=1}^{24} M_{c,ingest,0,i} \quad (186)$$

$$ind.ingest.abs = \sum_{i=1}^{24} M_{c,ingest,abs,i} \quad (187)$$

where:

ind.ingest.exp	=	daily mass of chemical ingested due to indirect exposure [mg]
$M_{c,ingest,0,i}$	=	hourly mass of chemical ingested due to indirect exposure [mg]
ind.ingest.abs	=	daily mass of chemical absorbed into the gut due to indirect exposure [-]
$M_{c,ingest,abs,0,i}$	=	hourly mass of chemical absorbed into the gut due to indirect exposure [-]

9.4 Indirect inhalation exposure

9.4.1 General overview

The Indirect Exposure function currently uses average air concentration as a measure of indirect inhalation exposure. Two sources of indirect inhalation exposure are considered: evaporation of chemical into the air from the hands after contact with chemical-containing surfaces, and chemical transfer into air due to product use by all members of the household. To account for both sources of indirect inhalation exposure, an overall chemical concentration must first be calculated before metrics of inhalation exposure can be determined.

9.4.2 Evaporation of chemical into air from hands

The mass of chemical in the air resulting from dermal contact with chemical-containing surfaces is calculated following the same approach for indirect dermal absorption and indirect ingestion and is given below. As previously stated, the duration of indirect contact is assumed to be eight hours divided by the number of hand washes per day, and therefore a given fraction of dermal exposure is inhaled for every chemical, where the same fraction applies to all hours of the year which have any indirect contact.

$$M_{c,air,1} = M_{c,hands,0} \times f_{sk,evap} \times (1 - exp^{-k_{sk,lost} \times t}) \quad (188)$$

$$f_{sk,evap} = \frac{k_{sk,evap}}{k_{sk,lost}} = \frac{k_{sk,evap}}{k_{sk,abs} + k_{sk,evap} + k_{sk,oth} + k_{sk,hm}} \quad (189)$$

$$t = \frac{8}{hw} \quad (190)$$

where:

$M_{c,air,1}$	=	mass of chemical picked up on hands on current hour going to air [mg]
$M_{c,hands,0}$	=	initial mass of chemical on the hands [mg]
$f_{sk,evap}$	=	fraction of overall dermal loss due to evaporation from skin surface to air [-]
$k_{sk,lost}$	=	rate constant for overall dermal loss [h^{-1}]
$k_{sk,evap}$	=	rate constant for evaporation from skin surface to air [h^{-1}]
$k_{sk,abs}$	=	rate constant for absorption from skin surface into stratum corneum [h^{-1}]
$k_{sk,oth}$	=	rate constant for other removal from skin surface [h^{-1}]
$k_{sk,hm}$	=	rate constant for hand-to-mouth transfer [h^{-1}]

t = duration of indirect contact [h]
hw = number of handwashing events per day, varies by person [-]

The chemical concentration in air resulting from dermal contact with chemical-containing surfaces is calculated as shown below. The average air concentration is in addition to the background air concentration throughout the house, and is determined by balancing the rates of chemical inflow and outflow for the personal cloud. Assuming a personal cloud volume of 2 m^3 and an air exchange rate with the house (aer_{cloud}) of 10 hr^{-1}, then :

$$inflow = \frac{mass\ (mg)}{time\ (hr)} = M_{c,air,1} \times hw/8$$

$$outflow = C_{c,air,1} \times V_{cloud} \times aer_{cloud}$$

$$C_{c,air,1} = \frac{M_{c,air,1} \times hw}{V_{cloud} \times aer_{cloud} \times 8} \quad (191)$$

where:

$inflow$ = chemical inflow into the personal cloud [mg/hr]
$outflow$ = chemical out of the personal cloud [mg/hr]
$C_{c,air,1}$ = concentration of chemical in air due to evaporation from hands [mg/m^3]
$M_{c,air,1}$ = mass of chemical on hands due to contact with chemical-containing surfaces [mg]
V_{cloud} = personal cloud [m^3], assumed to be 2
aer_{cloud} = air exchange rate between the personal cloud and the house [hr^{-1}]
hw = number of handwashing events per day, varies by person [-]

9.4.3 Chemical present in air from previous product use

The mass of chemical transferred into air due to product use by all members of the household is obtained from the Fugacity function, which provides an hourly time series of chemical mass on indoor surfaces and in indoor air. In this model, the chemical from past product use is assumed to be uniformly dispersed throughout the house. The corresponding chemical concentrations are calculated based on house properties as follows:

$$C_{c,air,2} = \frac{M_{c,air,2}}{A_{house} \times h_{house}} \quad (192)$$

where:

$C_{c,air,2}$ = concentration of chemical in air due to past product use by all household members [mg/m^3]
$M_{c,air,2}$ = mass of chemical in air due to past product use by all household members [mg], taken from the Fugacity function

A_{house} = floor area of house [m^2]
h_{house} = average room height [m]

9.4.4 Overall chemical concentration and mass inhaled and absorbed

An overall chemical concentration can be calculated by aggregating the air concentrations resulting from the two sources of indirect inhalation exposure as follows:

$$C_{c,air,overall} = C_{c,air,1} + C_{c,air,2} \quad (193)$$

where:

$C_{c,air,overall}$ = overall concentration of chemical in air due to indirect exposure [mg/m^3]
$C_{c,air,1}$ = concentration of chemical in air due to evaporation from hands [mg/m^3]
$C_{c,air,2}$ = concentration of chemical in air due to past product use by all household members [mg/m^3]

Using the overall chemical concentration in air, three inhalation outputs can be determined for every hour: inhalation exposure, mass of chemical inhaled, and mass of inhaled chemical mass absorbed.

(i) Inhalation exposure. This is defined as the concentration of chemical due to indirect exposure sources that the primary individual is exposed to. As stated in Section 9.1, inhalation exposure only occurs during two exposure periods, when the person is awake at home or asleep at home. Accordingly, inhalation exposure is calculated as the overall air concentration weighted by the fraction of the hour spent at home.

$$C_{c,air,exp} = C_{c,air,overall} \times f_{home} \quad (194)$$

$$f_{home} = \frac{t_{awake} + t_{asleep}}{60} \quad (195)$$

where:

$C_{c,air,exp}$ = concentration of chemical from indirect sources that the primary individual is exposed to [mg/m^3]
$C_{c,air,overall}$ = overall chemical concentration in air from indirect sources [mg/m^3]
f_{home} = fraction of the hour spent at home [-]
t_{awake} = minutes in an hour spent awake at home [min]
t_{asleep} = minutes in an hour spent asleep at home [min]

(ii) Mass of chemical inhaled. This is mass of chemical inhaled due to indirect exposure when the primary person is asleep and awake at home. It is calculated based on the basal or baseline breathing ventilation rate (i.e., when a person is lying down) and assuming a metabolic energy multiplier (met) of 2.2 when the primary individual is awake at home.

$$M_{c,air,inhal} = \left(C_{c,air,overall} \times \frac{f_{asleep}}{60} \times r_{vent}\right) + \left(C_{c,air,overall} \times \frac{f_{awake}}{60} \times r_{vent} \times met\right) \quad (196)$$

where:

$M_{c,air,inhal}$ = mass of chemical from indirect sources that is inhaled [mg]
$C_{c,air,overall}$ = overall chemical concentration in air from indirect sources [mg/m^3]
r_{vent} = basal ventilation rate [m^3/day]
met = metabolic energy multiplier [-], assumed to be 2.2
f_{awake} = fraction of hour spent awake at home [min]
f_{asleep} = fraction of hour spent asleep at home [min]

(iii) Mass of inhaled chemical absorbed. This is calculated as follows assuming 16% of the mass inhaled is absorbed into the blood.

$$M_{c,inhal,abs} = M_{c,air,inhal} \times f_{inhal,abs} \quad (197)$$

where:

$M_{c,air,inhal,abs}$ = mass of chemical absorbed into the blood through inhalation [mg]
$M_{c,air,inhal}$ = mass of chemical from indirect sources that is inhaled [mg]
$f_{inhal,abs}$ = mass fraction absorbed into the blood [-], set to 0.16

9.4.5 Output metrics

To calculate daily inhalation metrics (Table 2), the average hourly concentration the primary individual is exposed to, mass of chemical inhaled, mass of chemical absorbed, and the maximum hourly air concentration, can be calculated as shown below. For simplicity, these post-contact exposures are assigned to the same hour as the initial contact.

$$ind.inhal.exp = \frac{\sum_{i=1}^{24} C_{c,air,exp,i}}{24} \quad (198)$$

$$ind.inhal.mass = \sum_{i=1}^{24} M_{c,air,inhal,i} \quad (199)$$

$$ind.inhal.abs = \sum_{i=1}^{24} M_{c,air,inhal,abs,i} \quad (200)$$

$$ind.inhal.max = \max(C_{c,air,overall,i}) \quad (201)$$

where:

ind.inhal.exp = average hourly chemical concentration the primary individual is exposed to [mg/m^3]

$C_{c,air,exp,i}$	=	hourly concentration of chemical the primary individual is exposed to [mg/m^3]
ind.inhal.max	=	daily mass of chemical inhaled due to indirect exposure [mg]
$M_{c,air,inhal,i}$	=	hourly mass of chemical inhaled due to indirect exposure [mg]
$M_{c,inhal,abs,daily}$	=	daily mass of chemical absorbed into the gut due to indirect exposure [mg]
ind.inhal.abs	=	hourly mass of chemical absorbed into the gut due to indirect exposure [mg]
ind.inhal.max	=	maximum hourly air concentration per day due to indirect exposure [mg/m^3]
$C_{c,inhal,exp,daily}$	=	hourly air concentration due to indirect exposure [mg/m^3]

10. Environmental Impact function: eval.env.impact()

The Environmental Impact function estimates the chemical masses contributed to the environment by the activities of the household through both indoor and outdoor disposal methods. Daily totals are sufficient at all times.

Inputs

nc diary	activity diaries of all the individuals in the household, output from the Product Use scheduler module
use.data	chemical masses with one dimension each for the number of PUCs being used by the household, the use phase, number of compartments to which the PUC releases chemical to, and the number of chemicals in the representative product and formulation of the PUC that has been randomly chosen for the household
pucs	only those PUCs that are also part of the house diary (for any specific house being evaluated in the loop over houses), with related information, for example, the unique PUC identifier code
fug.day	daily masses of chemicals in the indoor air, indoor surface, out-the-window and waste compartments after applying the fugacity calculations
compart.list	names of the 11 compartments that are being modeled as part of the mass partition approach
chem.totals	total annual household usage (mg) of each chemical
nc	number of chemicals being modeled in the current model run

Outputs

env.impact	daily masses of chemicals (mg) released by the household (Table 2) into the outdoor air (out.air), outdoor surface (out.sur), the drain (drain), and the solid waste (waste) compartments

10.1 Contributions to the environment

There are four compartments of interest considered in S2D: drain, waste, outdoor air, and outdoor surfaces.

1. Drain includes everything washed down the sinks and drains, which enters the sewage treatment system.

2. Waste includes things placed in the trash and picked up by garbage trucks. Two contributions to waste are considered. The "direct" contribution is from the "waste" compartment at the end of active product use (see Section 6). The "indirect" waste component is from the cleaning terms in the fugacity calculations (see Section 7) where it is assumed that cleaning primarily involves vacuuming or sweeping dust, which is discarded in the trash.

3. Outdoor air has two components: products used outdoors, and indoor air that moves outdoors by air exchange in the fugacity model.

4. Outdoor surfaces include products used outdoors.

10.2 Estimates of environmental releases

As indicated above, contributions to the environment occur as a result of direct product use and from fugacity calculations. From direct product use, the mass of chemical in the outdoor air, outdoor surfaces, drain, and waste components are evaluated on a per-product-use basis. Daily estimates of chemical mass for each of the four compartments are calculated using the diary events output from the Product Use Scheduler module to identify when products are used, and summing up the contributions from each product use. From the fugacity calculations, a daily output of chemical release into outdoor air (as a result of indoor air that moves outdoors) and solid waste (from cleaning) is provided.

Chemical release estimates to each of the four environmental compartments is given below:

$$drain = \sum_{j=1}^{n} M_{c,drain,3,j} \tag{202}$$

$$waste = \sum_{j=1}^{n} M_{c,waste,3,j} + M_{c,fug,ws,daily} \tag{203}$$

$$out.air = \sum_{j=1}^{n} M_{c,oa,3,j} + M_{c,fug,oa,dailyi} \tag{204}$$

$$out.sur = \sum_{j=1}^{n} M_{c,os,3,j} \quad (205)$$

where:

drain	=	daily mass of chemical released down the drain [mg]
$M_{c,drain,3,j}$	=	mass of chemical released down the drain per product use [mg]
$M_{c,ws,dialy}$	=	daily mass of chemical released to waste [mg]
$M_{c,waste,3,j}$	=	mass of chemical released to waste per product use [mg]
waste	=	daily mass of chemical released to waste as a result of cleaning [mg]
$M_{c,oa,dialy}$	=	daily mass of chemical released to outdoor air [mg]
$M_{c,oa,3,j}$	=	mass of chemical released to outdoor air per product use [mg]
out.air	=	daily mass of chemical released to outdoor air due to air exchange with house [mg]
out.sur	=	daily mass of chemical released to outdoor surfaces [mg]
$M_{c,os,3,j}$	=	mass of chemical released to outdoor surfaces per product use [mg]
n	=	number of times product is used over the course of each day [-]

11. Summary functions

11.1 Chemical releases outdoors

The annual mass of chemical released to outdoor air, water, and land is calculated using the daily mass values. For release to land, contributions from waste and outdoor surfaces are considered.

The calculations for each of the three releases are given below:

$$M_{c,oa,annual} = 364 \times M_{c,oa,daily} \times \frac{M_{c,total,1o}}{M_{c,total,all}} \quad (206)$$

$$M_{c,water,annual} = 364 \times M_{c,dr,daily} \times \frac{M_{c,total,1o}}{M_{c,total,all}} \quad (207)$$

$$M_{c,land,annual} = 364 \times (M_{c,os,daily} + M_{c,ws,daily}) \times \frac{M_{c,total,1o}}{M_{c,total,all}} \quad (208)$$

where:

$M_{c,oa,annual}$	=	total annual mass of chemical released to outdoor air [mg]
$M_{c,water,annual}$	=	total annual mass of chemical released to water [mg]
$M_{c,land,annual}$	=	total annual mass of chemical released to land [mg]
$M_{c,oa,daily}$	=	daily mass of chemical released to outdoor air [mg]
$M_{c,dr,daily}$	=	daily mass of chemical released down the drain [mg]
$M_{c,os,daily}$	=	daily mass of chemical released to outer surfaces [mg]
$M_{c,ws,daily}$	=	daily mass of chemical released to waste (solid) [mg]

$M_{c,total,1o}$	=	total annual mass of chemical for the PUC due to use by the primary person use [mg]
$M_{c,total,all}$	=	total annual mass of chemical for the PUC due to use by all household members [mg]

11.2 Summary of daily and annual outputs: eval.summary()

The summary function writes daily and annual output files for each household.

Inputs (see sections on direct and indirect exposure functions and the environmental impact function for details as these inputs are outputs from those functions; see Table 2 for variable names and definitions)

direct	daily direct exposure metrics including the dermal exposure (mg), dermal maximum loading (mg/cm^2), dermal absorbed dose (mg), inhalation exposure (mg/m^3), inhaled mass (mg), maximum air concentration (mg/m^3), inhaled mass (mg), inhaled mass of chemical absorbed (mg), ingested chemical mass (mg), ingested chemical mass absorbed (mg) for each chemical
indirect	daily indirect exposure metrics including the dermal exposure (mg), dermal maximum loading (mg/cm^2), dermal absorbed dose (mg), inhalation exposure (mg/m^3), inhaled mass (mg), maximum air concentration (mg/m^3), inhaled mass (mg), inhaled mass of chemical absorbed (mg), ingested chemical mass (mg), ingested chemical mass absorbed (mg) for each chemical
env.impact	daily masses of chemicals released by the household into the outdoor air, outdoor surface, the drain and the solid waste compartments
Run.name	a character string of the run name
house.num	the ID of the household being evaluated
nc	number of chemicals being modeled in the current model run
chem.list	all the chemicals
chem.totals	total annual household usage (mg) of each chemical

Outputs

daily	list of all exposure metrics for each day of the year per household
annual	list of all exposure metrics for the entire year per household

11.3 Source-to-Dose summary report: eval.Summary()

The S2D Summary Function is a separate module that accompanies the S2D main code. The purpose of this function is to create a summary report of S2D outputs in .pdf format. The summary report includes mandatory and optional output variables, detailed in Tables 14 and 15.

Table 14. Mandatory variables in the S2D Summary Function output.

Variable name	Description of Output Variable
PrimaryHH	Data for primary person only in each household.
AllHH	Data for every person in each household under consideration.
DTXSID	DSSTox Chemical ID
Chemical.Name	Chemical name
CAS	CAS number
PUC	Product Use Category (alphanumeric code)
PUC_Name	Name of this PUC
PUC_U	Number of households that use this PUC
PUC_not	Number of households that don't use this PUC
P_O_PUC	Number of households where the primary person (and other household members) use this PUC.
NP_O_PUC	Number of households where the primary person doesn't use this PUC but other household members do.
Code	Product type category code used for mass partitioning approach in Source to Dose (S2D)
Description	Description of this PUC
E_P_M	Expected prevalence (%, reported as a decimal) for males over 12 years (adult males), from habits and practices input data
S_P_M	Subset prevalence (%, reported as a decimal) for males over 12 years (adult males) for households included in S2D run
E_P_F	Expected prevalence (%, reported as a decimal) for females over 12 years (adult females), from habits and practices input data
S_P_F	Subset prevalence (%, reported as a decimal) for females over 12 years (adult females) for households included in S2D run
E_P_Ch	Expected prevalence (%, reported as a decimal) for individuals 12 years and under (children), from habits and practices input data
S_P_Ch	Subset prevalence (%, reported as a decimal) for individuals 12 years and under (children) for households in S2D run

E_Freq	Expected frequency (year^{-1}) for users, from habits and practices input data
S_Freq	Subset user frequency (year^{-1}) for households in S2D run
E_Mass	Expected mass used (mg) for users, from habits and practices input data
S_Mass	Subset user mass used (mg) for households in S2D run
A_P_M*	Actual prevalence (%, reported as a decimal) for males over 12 years (adult males) from full population run through Product Use Scheduler
A_P_F*	Actual prevalence (%, reported as a decimal) for females over 12 years (adult females) from full population run through Product Use Scheduler
A_P_Ch*	Actual prevalence (%, reported as a decimal) for individuals 12 years and under (children) from full population run through Product Use Scheduler
A_Freq*	Actual average frequency (year^{-1}), from full population run through Product Use Scheduler
A_Mass*	Actual average mass used (mg), from full population run through Product Use Scheduler

* Note that these variables need not be produced each time the Summary Function is run (they can be run once for a large set of diaries output from the Product Use Scheduler).

Table 15. Optional variables in the S2D Summary Function output.

Variable name	Description of Output Variable
Dose and chemical released	In the Control File, users choose from any combination of 13 S2D output variables, listed below, to be included in the optional Summary Table
tot.abs.dose	Average total absorbed dose (mg) of chemical
der.abs.dose.tot	Average dermal absorbed dose total (mg) per chemical
der.abs.dose.dir	Average dermal absorbed dose from direct exposures (mg) per chemical
der.abs.dose.ind	Average dermal absorbed dose from indirect exposures (mg) per chemical
inh.abs.dose.tot	Average inhalation absorbed dose total (mg) per chemical
inh.abs.dose.dir	Average inhalation absorbed dose from direct exposures (mg) per chemical
inh.abs.dose.ind	Average inhalation absorbed dose from indirect exposures (mg) per chemical
ing.abs.dose.tot	Average ingestion absorbed dose total (mg) per chemical
ing.abs.dose.dir	Average ingestion absorbed dose from direct exposures (mg) per chemical
ing.abs.dose.ind	Average ingestion absorbed dose from indirect exposures (mg) per chemical
mass.down.drain	Average mass of chemical released going to drain system(s) (mg)
mass.out.window	Average mass of chemical released to outdoor air (mg)
mass.solid.waste	Average mass of chemical disposed in trash (mg)
Age.group	In the Control File, users choose from one of the three options listed below
child	Primary people who are ≤ 12 years old
adult	Primary people who are > 12 years old
both	All primary people (both adults and children)
AvgMean.AllPop	Population average of annual mean across population (absorbed mass in mg)
AvgMean.Users	Population average of annual mean of users only (absorbed mass in mg)
AvgMaxDaily	Population average of maximum daily dose (absorbed mass in mg)

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Appendices

A. Input files

All required input files for the S2D module are detailed below, with the exception of pophouse.csv (an output from the RPGen module detailing each household, their demographics, and physiologic variables for the primary person in the household), and the household product use diaries (output from the Product Use Scheduler module, detailing product usage by day and time for each member of the household, for one year). In each input file, the order of variables does not matter, as the code refers to each variable by the name in the column header. Variable names (i.e., column headers) are not case sensitive, as they are converted to all lower case when the files are read in. Extra variables may appear on any input file, in any position. Most are not detailed below, but those that are are identified as 'optional.' 'Synonym' and 'units' columns appear in each data dictionary, even if synonyms or units are unavailable for a particular variable. If 'units' is left blank, the variable is not measureable (i.e., a character or a sequence index); if 'units' is coded as [-], the variable is a dimensionless quantity.

chem.file

List of chemical properties relevant to the S2D calculations.

Variable	Status	Synonyms	Units	Description
dtxsid	required			Chemical identifier from DSSTox (with prefix "DTXSID" followed by numerals)
x	required			Unique number for each DTXSID which determines the chemical-specific offset used by the random number seed
mw	required	molwt	g/mol	Molecular weight
vp.pa	required	vp_pa, vapor	Pa	Vapor pressure
log.low	required	log_kow	[-]	Base 10 logarithm of the octanol-water partition coefficient
water.sol.mg.l	required	water_sol_mg_l, solub	mg/liter	Solubility in water
half.sediment.hr	required	half_sediment_hr	1/hr	Half-life of chemical in sediment
half.air.hr	Required	half_air_hr	1/hr	Half-life of chemical in air
kp	required		cm/hr	Permeability on skin
fabs	required		[-]	Absorption fraction in gut

chem.frac.file (i.e., composition)

Product composition in terms of chemical fractions in the released mass.

The default composition file provided with the S2D module includes multiple representative products per product category, and was generated using data from the CPDat database (Dionisio, Phillips et al. 2018). Some product categories may contain more representative products than others, dependent on availability of data. There are 100 different formulations for each representative product in the

composition file. This is often indicative of the raw quantitative composition data obtained as a range of values, or predicted through a model (Isaacs, Phillips et al. 2018). When the weight fraction of a chemical is provided as a range of values (typically on a product material safety data sheet), 100 generic formulations are generated by randomly drawing a value between the reported minimum and maximum values for each ingredient in a product. The weight fractions of this generic formulation are accepted if the sum of the generic weight fractions of all ingredients is less than 1, otherwise the formulation is rejected. This process is repeated until 100 accepted formulations are produced for each product. When the weight fraction of chemical is not provided (typically on a product ingredient list), 100 generic formulations are generated by performing a weight fraction prediction algorithm (Isaacs, Phillips et al. 2018) 100 times. When the raw composition data are available as point estimates for the weight fraction of each chemical, then the 100 formulations for that representative product are all identical.

Variable	Status	Synonyms	Units	Description
source.id	required	id, shedsid		Unique PUC code (e.g. AC.0500.010.050.F)
product_id	required			Numeric identifier for representative product
formulation_id	required			Numeric identifier for specific formulation of the representative product
dtxsid	required			Chemical identifier (DSSTox unique identifier)
weight_fraction	required		[-]	Fraction of consumer product mass made up by the chemical

compart.file

The initial distribution of mass into compartments when the product is used.

Variable	Status	Synonyms	Description
code	required	cod	3-letter code for compartment fractions category
description	required	des	Description of code category
fia: indoor air	required	fia	Fraction of product mass going to indoor air
fis: indoor surfaces	required	fis	Fraction of product mass going to indoor surfaces
fdr: drain	required	fdr	Fraction of product mass going down drain
fws: waste	required	fws	Fraction of product mass going to waste (trash)
fsk: skin	required	fsk	Fraction of product mass going directly to skin
foa: outdoor air	required	foa	Fraction of product mass going to outdoor air
fos: outdoor surfaces	required	fos	Fraction of product mass going to outdoor surfaces
fap: appliances	required	fap	Fraction of product mass going into appliances
fsl: solid	required	fsl	Fraction of product mass remaining indefinitely in house
fgi: gi	required	fgi	Fraction of product mass going to gastrointestinal tract
fhn: hair_nails	required	fhn	Fraction of product mass going on to hair and nails
sum	optional		Sum of 11 fractions

indoor	optional	ind	Flag: 1=indoor use, 0=outdoor use

fug.file

Distributions of house-specific variables relevant to chemical redistribution by the fugacity calculations.

Variable	Status	Description
Varname	required	Name of variable as used in S2D code
Form	required	Type of distribution
Par1	required	First distributional parameter
Par2	required	Second distributional parameter (if needed, dependent on form)
Par3	required	Third distributional parameter (if needed, dependent on form)
Par4	required	Fourth distributional parameter (if needed, dependent on form)
lower.trun	required	Lowest possible value
upper.trun	required	Highest possible value
resamp	required	Flag: yes=resample when out of bounds, no=set to bound
units	optional	Units for the S2D variable
description	optional	Description of the S2D variable

puc.met.file

Mean MET values (which determine inhalation rate) during product use, for each PUC.

Variable	Status	Synonyms	Units	Description
source.id	required	new_puc		Unique PUC code (e.g. AC.0500.010.050.F)
mean mets from APEX	required		[-]	Mean MET value for time spent using this PUC
new_general_category	required			General PUC category
new_product_type	required			Product type
new_refined product type	required			Refined product type
chad activity	required			CHAD activity code from which MET value was derived
old_PUC	optional			Old PUC product code (i.e., SHEDS-HT product code)

puc.type.file

The 2-letter code for each PUC which determines which set of compartment fractions to use.

Variable	Status	Synonyms	Description
source.id	required	new_source.id	Unique PUC code (e.g. AC.0500.010.050.F)
code	required		3-letter product code used with compartment fractions

removal.file

Rates of removal by wiping or rinsing at the end of product use, for each PUC.

Variable	Status	Synonyms	Units	Description
source.id	required	new_puc		Unique PUC code (e.g. AC.0500.010.050.F)
fhands	required		[-]	Fraction of product mass applied to skin that goes to hands
fbody	required		[-]	Fracion of product mass applied to skin that goes to rest of body (excluding hands)
frinseh	required		[-]	Fraction of mass on hands rinsed off at end of product use (going to drain)
frinseb	required		[-]	Fraction of mass on body rinsed off at end of product use (going to drain)
frinses	required		[-]	Fraction of mass on surfaces (not the skin) rinsed off at end of product use (going to drain)
fwipeh	required		[-]	Fraction of mass on hands wiped off at end of product use (going to waste)
fwipeb	required		[-]	Fraction of mass on body wiped off at end of product use (going to waste)
fwipes	required		[-]	Fraction of mass on surfaces (not the skin) wiped off at end of product use (going to waste)

skin.area.file

Skin area fractions that may obtain chemical loading, for each PUC.

Variable	Status	Synonyms	Units	Description
source.id	required	new_puc		Unique PUC code (e.g. AC.0500.010.050.F)
child	required		[-]	Fraction of skin area affected by this PUC (for children)
adult	required		[-]	Fraction of skin area affected by this PUC (for adults)
hand_variability	required			Variabiltiy category for fracitonal hand area affected: high, medium, or low
body_variability	required			Variability category for fractional body area affected: high, medium, or low

vent.file

Distributional parameters for basal breathing ventilation rate, by age and gender.

Variable	Status	Units	Description
sex	required		Sex: M=male, F=female
minage	required	years	Minimum age to use this distribution
maxage	required	years	Maximum age to use this distribution
mean_ve	required	m^3/day	Mean basal ventilation rate

std_ve	required	m^3/day	Standard deviation (across persons in this group) of basal ventilation rate