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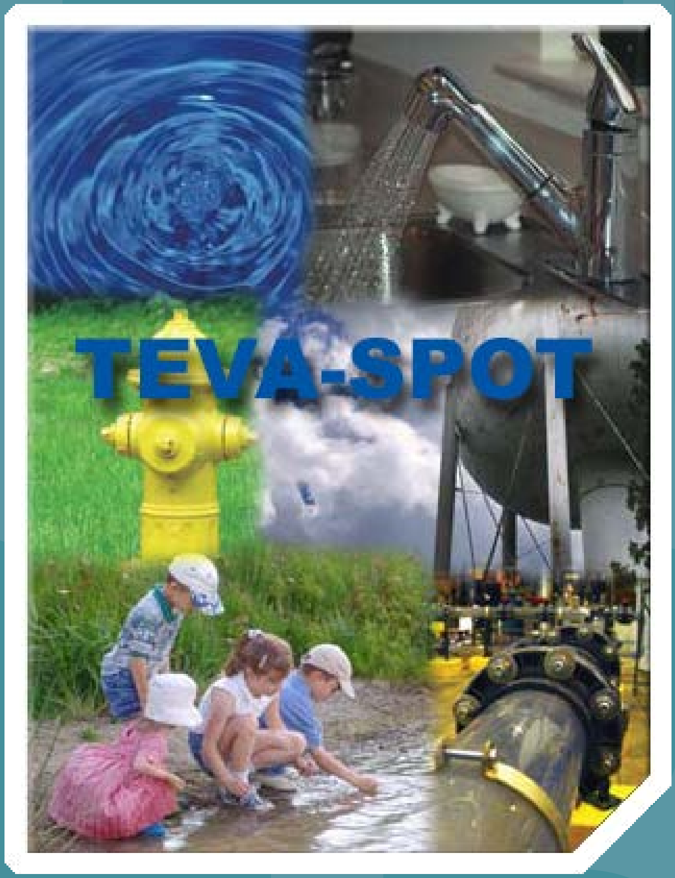
Incorporating a Capability for Estimating Inhalation Doses in TEVA-SPOT



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United States Environmental Protection Agency
Office of Research and Development
National Homeland Security Research Center
Cincinnati, Ohio 45268

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Disclaimer

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1 Introduction

Various uses of water have the potential to result in exposures to contaminants present in the water via the inhalation pathway. Contaminants can be present in aerosols generated during water use; volatile contaminants can be released to the air by such use. Considerable effort has been devoted to studying chronic exposures to volatile contaminants in drinking water. Aerosol production associated with water use has also been studied; the motivation again has been chronic exposures to contaminants. A detailed examination of chronic inhalation exposures to contaminants in drinking water has been provided in a monograph edited by Olin (Olin 1999).

During contamination events in a water distribution system (WDS), the potential exists for short-term inhalation exposures to elevated concentrations of contaminants. Such acute exposures have not received the same attention as has been devoted to chronic inhalation exposure to contaminants such as disinfection byproducts. In particular, there do not appear to be any studies of the system-wide inhalation exposures that could occur during a contamination event in a WDS. Various domestic uses of water can release volatile contaminants or generate aerosols or do both. The largest inhalation exposures to volatile contaminants likely result from showering (Wilkes et al. 1992). A screening-level assessment of inhalation exposure doses indicates that ultrasonic and cool-mist humidifiers and showering likely are the largest sources of exposures to contaminants contained in aerosols (Hines et al. 2014).

This report presents the approach (the software design) that was used to incorporate inhalation models in the U.S. Environmental Protection Agency's Threat Ensemble Vulnerability Assessment, Sensor Placement Optimization Tool (TEVA-SPOT) (U.S. EPA 2015). The software design outlined here and incorporated into TEVA-SPOT provides the capability for estimating inhalation doses that result from the most important sources of contaminated aerosols and volatile contaminants during a contamination event. TEVA-SPOT has had the capability to provide estimates of ingestion doses associated with a contamination event for the population served by a WDS. The approach presented here now provides TEVA-SPOT with a comparable capability for inhalation exposures. This report does not provide derivations of equations, attempt to justify use of specific values for parameters, or provide any recommendations for users of the approach. These are all subjects that will be addressed more appropriately elsewhere. The purpose of this report is two-fold: (1) to document the inhalation models that have been incorporated in TEVA-SPOT and (2) to provide some brief background for the models.

In the approach used in TEVA-SPOT, individuals using water from a distribution system are located at the nodes (junctions) in the system at which there is a nonzero demand for water. Contaminant concentration during a contaminant event is determined at all system nodes using EPANET (Rossman 2000). Concentration varies with time and location during an event. Consequently, the behavior of individuals with respect to how they use water is important because it determines the times at which possible exposures to contaminated water can occur. Inhalation doses for individuals that result from exposures to contaminated water can be determined using the approach presented in this document. These individual doses can then aggregated to obtain system-wide results.

Section 2 discusses the approach implemented in TEVA-SPOT for estimating inhalation doses for showering. Section 3 presents the approach used for estimating inhalation doses from humidifier use. Section 4 discusses some additional calculations that apply to both showering and humidifier use. References are provided at the end of the document.

2 Showering

2.1 Introduction

Including a capability for estimating inhalation doses associated with showering in TEVA-SPOT requires a model for showering behavior and a model for estimating contaminant concentrations in the air in a shower. Contaminants may be present in the air in a shower due to the release of volatile contaminants contained in the shower water or the formation of aerosol particles by the shower head. In either case, the air concentration in a shower will vary with time approximately as shown in Fig. 1. The air concentration will tend to approach an equilibrium value if the shower is on for sufficient time and will decrease when the shower is turned off. The equilibrium concentration is determined by the relative sizes of the source and loss rates for the contaminant. Contaminant mass can be lost due to air exchanges between the shower stall and the adjacent room and by deposition and other processes.

Inhalation dose is determined by the air concentration of the contaminant in the shower, the length of time an individual remains in the shower while it is on, the length of time an individual remains in the shower after it is turned off, and the individual's breathing rate. Air concentration is determined by contaminant concentration in the water entering the shower and the physical processes affecting the generation and loss of the contaminant in the air in the shower stall. Water concentration is determined by the concentration in the distribution system, which varies with time. Estimating the inhalation dose for an individual requires specifying the behavior of the individual, namely the frequency at which showers are taken, the times when they are taken, and their duration.

Models for behavior that describe showering frequency, duration, and timing are outlined and discussed in Sections 2.2 - 2.4, followed in Section 2.5 by a presentation of approaches for estimating inhalation doses based on several models for the physical processes that determine the air concentrations of a contaminant in a shower.

The following discussion outlines how inhalation doses are determined for individual receptors who shower using water from a distribution system. Results for individual receptors are aggregated by scenario and ensemble as is already done in TEVA-SPOT for ingestion dose.

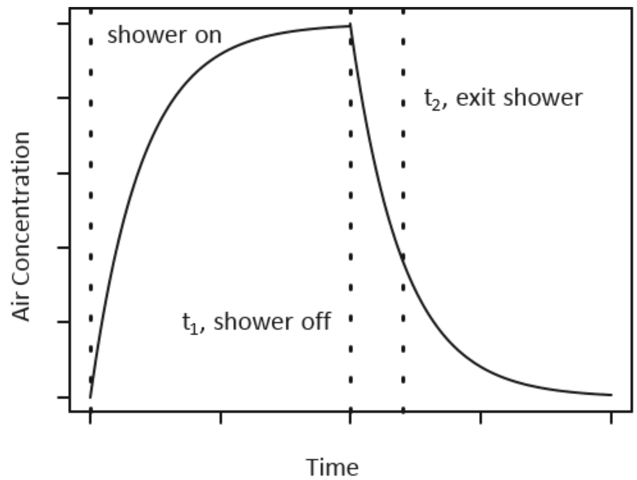

Figure 1: Air Concentration of Contaminant in a Shower. The vertical dotted lines indicate when the shower is turned on, turned off, and when the individual exits the shower.

2.2 Behavior: Background

Given the limitations in available data, a number of assumptions are necessary when developing a model that includes showering frequency, duration, and timing. In particular, the major assumptions are the following: (1) showering duration is independent of showering frequency and timing; (2) the behavior of each individual is the same for each day in a simulation; and (3) the timing of grooming events as reported in time-use studies serve as an adequate proxy for the timing of showering events. Because less than 1% of the population takes more than two showers per day (Wilkes et al. 2005), it will be assumed that all individuals take two or less showers per day. Finally, because we generally have no demographic information on the individuals at receptor locations (the network nodes), we do not consider how any parameters might vary with demographic factors such as age or gender.

The approach used in TEVA-SPOT to account for receptor behavior associated with showering is similar to that used to account for behavior related to ingestion of tap water. However, the model used for ingestion of tap water has only two parameters involving behavior, namely timing and volume; the model used for inhalation requires three. Each individual at each network node needs to be assigned a daily number of showers (0, 1, or 2). If an individual is assigned one or more showers, values for shower duration and starting time(s) also need to be assigned.

Estimates for showering frequency and duration are available (Wilkes et al. 2005). The American Time Use Survey (ATUS 2013) provides data on when grooming events occur. These events include showering, which is a major subset of grooming activity. The occurrence of grooming events sets bounds on when showering can occur, but not all grooming events involve showering.

Wilkes et al. (2005) provide results only for the length of time a shower is turned on. No similar results appear to be available for the length of time an individual spends in the shower stall after the shower is turned off. This quantity has a default value of zero, but can be provided by the user, if desired.

2.3 Behavior: Approach

A detailed model for behavior is presented in this section. Options included in TEVA-SPOT for modeling behavior are presented in Section 2.4 and also include more simplified models.

2.3.1 Showering Frequency

Showering frequency is determined using results presented in Table II of Wilkes et al. (2005), which are based on the analysis of data from the National Human Activity Patterns Survey. Considering individuals of all ages, for the day of the survey 22% reported not taking a shower, 60% reported taking one shower, and 18% reported taking two or more showers. (As noted above, less than 1% take more than two showers per day.) The showering frequency to assign to each individual at each node is determined by drawing a random number from U(0,1). If the number does not exceed 0.22, the individual does not shower. If the number is greater than 0.22 but does not exceed 0.82, the individual takes one shower per day. If the number exceeds 0.82, the individual takes two showers per day. Showering frequency is the same for each day in a simulation. An option is provided that allows frequencies to be specified by the user.

2.3.2 Showering Duration

Showering duration is determined using the results presented in Table V or Fig. 4 of Wilkes et al. (2005) that were developed by analyzing data from the Residential End Uses of Water Survey. From this source the distribution of showering durations is approximately lognormal. On a logarithmic scale the parameters for the distribution are μ = 1.92 and σ = 0.493. (Given in minutes, they would be exp(1.92) = 6.8 and exp(0.493) = 1.64.) The showering duration for an individual is determined by drawing a random number from a lognormal distribution with these parameters. To avoid a possibility of very long showering durations, any duration that exceeds 60 min is assigned a value of 61 min. (For the distribution being used, the probability that the showering duration will exceed 60 min is less than 0.0001.) Showering duration is assumed to be the same for both showers if an individual takes two showers per day and is assumed to remain the same for each day in a simulation.

2.3.3 Showering Start Times

Estimates for showering start times are determined using results obtained from ATUS for the timing of grooming. For individuals taking one shower per day, a starting time is obtained using an empirical probability distribution based on ATUS timing data for grooming. When a second shower is taken, its timing is influenced by the time of the first shower. To avoid issues related to trying to account for this dependency using probability distributions, random samples are taken of actual reported starting times for events in ATUS data. Starting times for an individual remain the same for all days in a simulation. No information is available on the time delay between the start of a grooming event and the start of a shower. It is assumed to be zero.

One Event:

Fig. 2 shows the empirical, weighted cumulative distribution for starting times for single grooming events for 2003-2012 ATUS data. It is based on the 54,094 events reported by the 54,094 individuals reporting one grooming event.

A text file ("cdf2003-12singles.txt" and included with this report), was developed using ATUS data, that contains tab-separated values for the starting times and cumulative probabilities plotted in Fig. 2. There are 101 rows in the file. The first entry in each row is the cumulative probability (0 to 1.0) and the second entry is the corresponding starting time (0.0 to 24.0 hours).

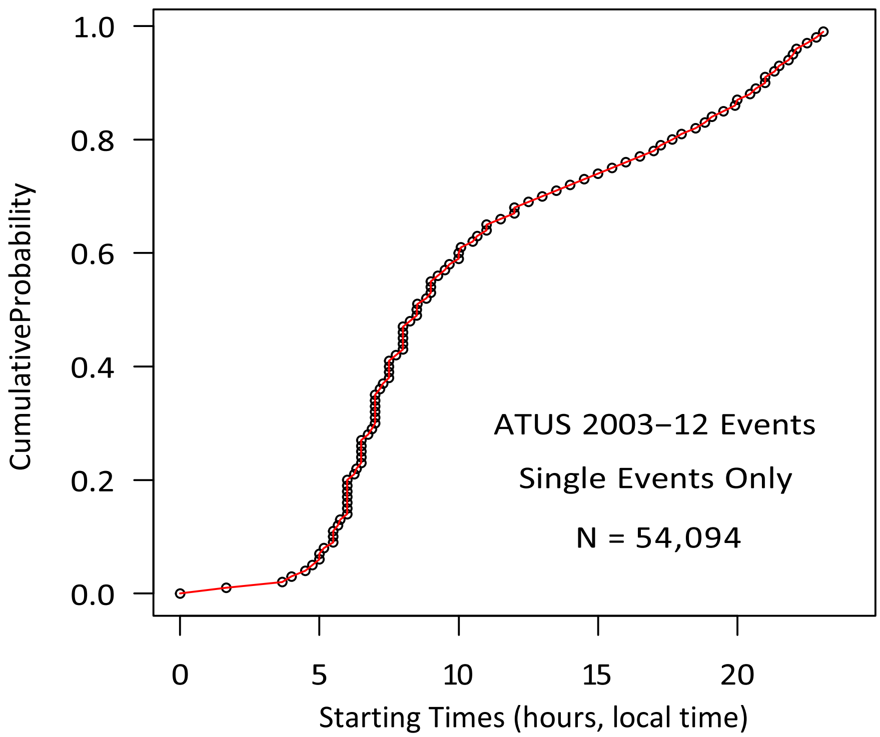

Figure 2: Cumulative Distribution of Starting Times for Single Showering Events

In TEVA-SPOT, random starting times are determined by inversion using the results plotted in Fig. 2 and contained in the text file. Inversion is accomplished by fitting a spline function (call it g) to the values for starting time (T) and cumulative probability (P) in Fig. 2, so that $T = g(P)$. A random starting time, t, is given by $t = g(p)$, where p is a random number drawn from U(0,1). t is distributed according to the empirical distribution in Fig. 2. Random starting times are determined in this way for all individuals at all nodes who have one showering event per day.

Two Events:

A second text file ("two events 2003-12.txt" and included with this report) was developed that contains data for all 36,652 ATUS respondents who reported two grooming events in 2003 to 2012. Results in this file are used in TEVA-SPOT to generate random starting time for individuals who take two showers per day. The file has 36,652 rows and five tab-separated columns. The first column contains the year the data were collected and the second column contains the ATUS identifiers used for the respondents. The third column contains the starting times in hours local time for the first event and the fourth column contains the starting time in hours local time for the second event. The fifth column provides the ATUS weights for the respondents. Weights are needed to compensate for the manner in which sampling and data collection were carried out in ATUS. For example, some demographic groups were oversampled to ensure an adequate sample size and more sampling was done on weekends than weekdays. Response rates varied by demographic group and day of the week. The weight for a particular respondent is the number of person-days that the results for the respondent represent in the entire U.S. population. The total number of person-days for the U.S. is the size of the U.S. population multiplied by the number of days in a year.

For some respondents the starting time for the second event is numerically smaller than the starting time for the first. For example, the time of the first event could be 10:00 hours and the time of the second event could be 1:00 hours. Such cases occur when the second event begins after 24:00 hours. The survey period was from 04:00 hours on the first day for which respondents provided information to 04:00 hours on the second. In cases in which the starting time of the second event is numerically smaller than the starting time of the first event, the order of the events is reversed when assigning starting times.

Estimated weighted densities for starting times for the events included in the file are shown in Fig. 3. The figure is provided for illustration purposes only; the two distributions are not independent.

Weights for respondents can vary substantially. The ratio of the maximum to minimum weights in the file is about 251. Consequently, consideration of the weights is important when results in the file are used.

Weighted sampling with replacement is used to obtain starting times for individuals who take two showers per day. Starting times for two events for an individual are obtained by randomly selecting one of the 36,652 cases in the file, considering the weights for the cases. Sampling is done with replacement when more than one individual is considered.

The distribution of the time separation between events for cases with two events is shown in Fig. 4. The maximum separation between events is 12 hours. For more than 81% of the cases the separation between events is 6 hours or longer. However, in some cases the difference between reported starting times for the two events can be small. Of the 36,652 cases with two events, 24

(0.07%) have a time separation of 5 min or less, 73 (0.2%) have a time separation of 10 min or less, 164 (0.4%) have a time separation of 15 min or less, 514 (1.4%) have a time separation of 30 min or less, and 1,186 (3.2%) have a time separation of 60 min or less.

To avoid cases in which time separations are smaller than seems realistic for the time separating two showers, or in which the time difference is smaller than the shower duration, an option has been included that allows users to reject any cases in the data file in which the time separation is less than some specified value (e.g., 0.5 or 1.0 hours).

2.4 Behavior: Options

TEVA-SPOT allows users to choose among various options for ingestion behavior; to provide similar flexibility for considering inhalation exposures, several options related to inhalation are also provided. Using a label similar to those used for ingestion, the most detailed option is PD[1], for which the timing is specified by a probabilistic model, as is the duration. The simplest option, FM, has a fixed time (or times for individuals taking two showers) and a fixed duration. The intermediate option, FD, has a fixed time(s) and a duration described by a probabilistic model. For PD[1], the models for durations and times are described in Sections 2.3.2 and 2.3.3, respectively. For FD, the model for duration is described in Section 2.3.2. The time for a shower for individuals taking one shower is either 06:30 or 21:30 hours local time. These times are the most common times when people who take one shower per day actually shower (on the basis of estimated peaks in the weighted histograms for starting times for grooming events). For individuals taking one shower, 70% take it at the first time and 30% take it at the second time (on the basis of the fraction of individuals taking showers in the intervals from 02:00 to 14:00 hours and from 14:00 to 02:00 hours, respectively). For individuals taking two showers, the most common times are also 06:30 and 21:30 hours local time. For option FM, the times for showers are the same as for FD; the duration for all showers is 7.7 min, the average shower duration.

The approaches used in TEVA-SPOT for the three options for behavior are summarized in Table 1. For each individual, behavior is the same for all days in a simulation. The only parameters that a user can supply for the behavior models are shower frequencies and the minimum time separation between two showering events. Selection of an option (e.g., PD) for behavior is always required.

2.5 Estimating Doses

Contaminants may be present in shower air contained in aerosols or as a gas. For aerosols, a mass-balance model and an empirical model for estimating doses are available in TEVA-SPOT. These models are discussed in Section 2.5.1. For volatile contaminants, two approaches based on mass balance are available, one using a mass-transfer-coefficient model and the other a

[1]PD, FM, and FD are labels, not abbreviations. The first letter indicates whether the timing model is probabilistic (P) or uses a fixed time (F). The second letter indicates whether the duration model is probabilistic (D) or uses a fixed duration (M).

transfer-efficiency model. These are discussed in Section 2.5.2. Volatile chemical contaminants may be present as a gas and chemical, biological, and radiological contaminants may be contained in aerosols. If a chemical has even low volatility, the contribution of the portion of the mass of the chemical present in aerosols generated during showering to total inhalation dose can be neglected.

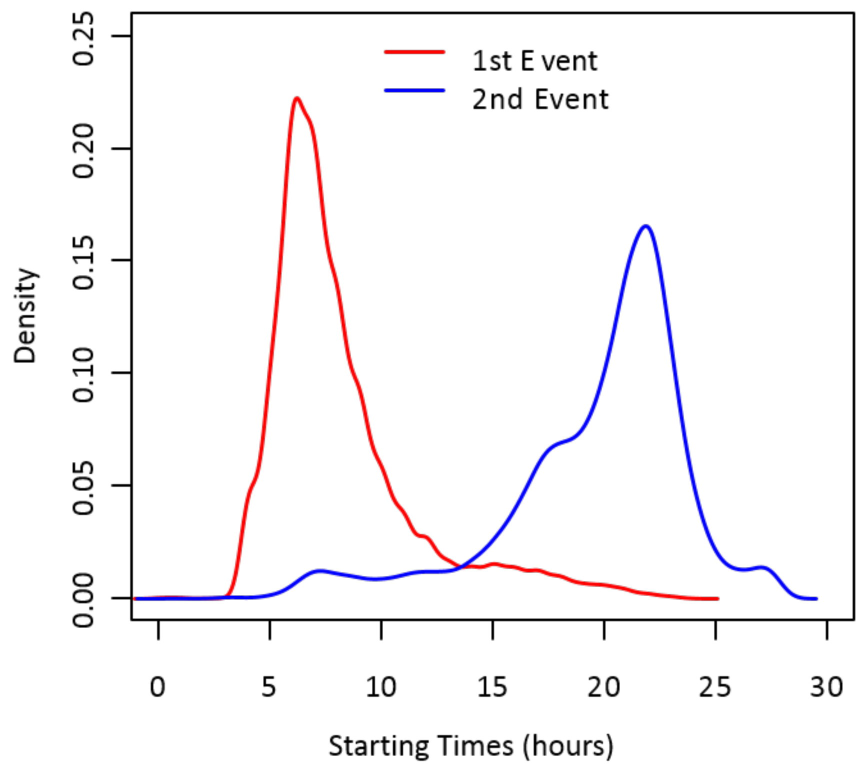

Figure 3: Estimated Weighted Probability Densities of Starting Times for Individuals with Two Showering Events (note that the two distributions are not independent and this figure is provided for illustration only). For cases in which the starting time of the second event is numerically smaller than the starting time of the first event, 24 hours was added to the starting time of the second event before densities were determined.)

Using models for the physical processes affecting contaminants in a shower, air concentrations of a contaminant in a shower stall were determined separately for aerosols and volatile chemicals. These concentrations were integrated over the duration of a shower and combined with an average breathing rate to obtain the estimates for inhalation dose presented here and available in TEVA-SPOT. These doses are the mass of the contaminant that enters the body by inhalation and are actually potential inhalation doses because not all of the contaminant mass will necessarily remain in the body; some is exhaled.

Doses are determined separately for each showering event and for each receptor because contaminant concentration varies with time during a simulation. Doses for each of the separate showering events for each individual receptor are added to obtain a cumulative dose for each receptor for the period of the simulation. These cumulative results for individual receptors can be binned, as is done for ingestion doses, so that the number of receptors with cumulative inhalation doses in each bin specified by the user are available for each scenario evaluated. Alternatively, dose-response data for a particular contaminant can be provided to TEVA-SPOT to allow estimation of health-effect end points. Section 4 discusses a capability that has been added to TEVA-SPOT that allows the user to determine the relative contribution of the most important showering event for each individual to the cumulative inhalation dose for the individual. This capability allows the user to examine the degree of conservatism involved in using cumulative doses.

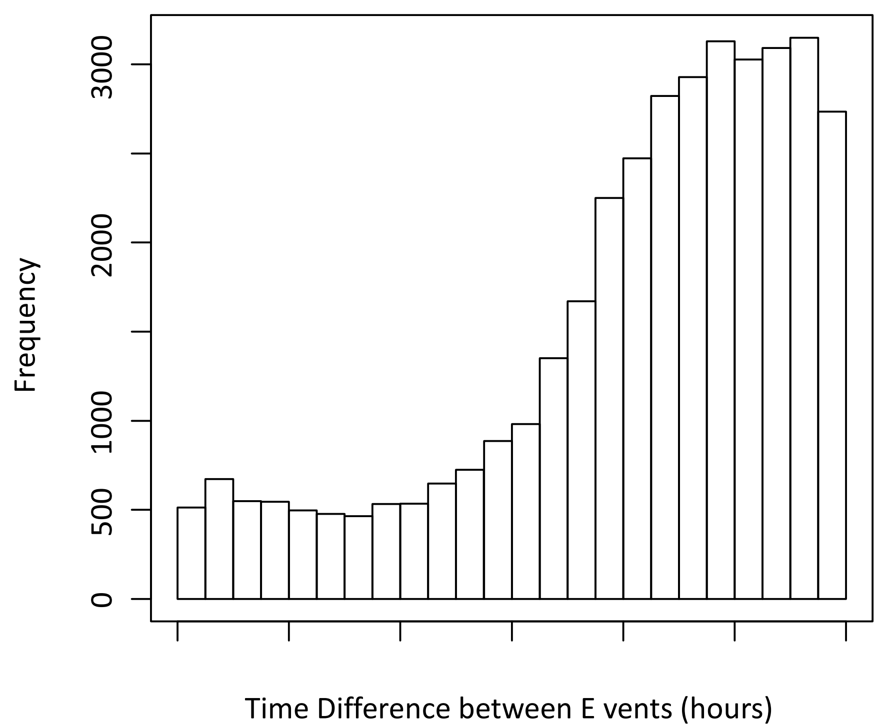

Figure 4: Histogram for Time Separation between Showering Events for Cases with Two Events (N = 36,652)

2.5.1 Aerosolization

The more detailed model for aerosolization is based on transient mass balance and requires the user to specify an empirically determined value for aerosol generation rate. The user also may specify an air exchange rate for the shower stall. Rates for other removal processes (e.g., settling or impaction) can be included in the value used for air exchange rate. The second model for aerosolization uses a purely empirical constant to relate contaminant concentration in the air to contaminant concentration in the water entering the shower.

Table 1. Summary of Options for Showering Behavior

Option[a]	Parameter	Model or values for parameter
All	Shower frequency	60% take one per day, 18% take two per day, 22% take none. User can specify frequencies
PD, FD	Shower duration	~ L(μ = 1.92, σ = 0.493), with any durations greater than 60 min set equal to 61 min
FM	Shower duration	7.7 min
PD	Times - one event	CDF in Fig. 2
PD	Times - two events	Sample times of actual events User can specify minimum time separation, if desired; default separation = 0
FD, FM	Times - one event	06:30 (70%) or 21:30 (30%) hours, local time
FD, FM	Times - two events	06:30 and 21:30 hours, local time

[a]PD, FM, and FD: The first letter indicates whether the timing model is probabilistic (P) or uses a fixed time (F). The second letter indicates whether the duration model is probabilistic (D) or uses a fixed duration (M).

Mass-Balance Model:

The mass-balance model assumes complete, immediate mixing of the contaminant in the air in the shower stall. Contaminant concentration in the shower air as a function of time was estimated using an approach similar to that used in Zhou et al. (2007). This time-varying concentration was integrated to give the inhalation dose, *D*, (in mg or number of cells [#]) for one showering event:

$$D = BGf/(k_1 V_s)\left[T_s - \frac{1}{k_1}(1 - exp(-k_1 T_s)) + \frac{1}{k_2}(1 - exp(-k_1 T_s))(1 - exp(-k_2 T_2))\right] \tag{1}$$

where *B* is the breathing rate (m^3/min), *G* is the aerosol mass generation rate (mg/min), *f* is the mass or number fraction of the contaminant in the water (see discussion below), V_s is the volume of the shower stall (m^3), k_1 is the removal rate for aerosols (min^{-1}) while the shower is on, T_s is the duration of the shower (min), T_2 is the time an individual remains in the shower after it is turned off (min), and k_2 is the removal rate for aerosols (min^{-1}) after the shower is turned off. The removal rates k_1 and k_2 are equal to the sum of the air exchange rate for the shower stall and the loss rate of particles due to deposition and other processes. In general, values for the various rates will depend on whether the shower is on or off.

If $T_2 = 0$, Eq. 1 reduces to the following:

$$D = \frac{BGf}{k_1 V_s}[T_s - \frac{1}{k_1}(1 - exp(-k_1 T_s))] \tag{2}$$

If $k_1 = k_2$ and $T_2 > 0$, Eq. 1 reduces to the following:

$$D = \frac{BGf}{k_1 V_s}\left[T_s - \frac{1}{k_1}(1 - exp(-k_1 T_s))(exp(-k_1 T_2))\right] \tag{3}$$

Contaminant air concentration in the shower stall is proportional to the aerosol mass generation rate (G), which determines the mass of aerosols in the air. Only a fraction of this aerosol mass is contributed by the contaminant; this fraction is f, the fraction of the water mass that is contaminant. It is assumed that the fraction of aerosol mass that is contaminant is the same as the fraction of incoming water mass that is contaminant. If the contaminant concentration in the shower water is 1 mg/L, then $f = 10^{-6}$ and has no units. If the contaminant in the shower water is an organism or spore, then f is the number of organisms or spores per milligram of shower water. If the concentration of organisms or spores in the shower water is 1 per L, then, since 1 L has a mass of 1 kg, $f = 10^{-6}$ mg^{-1}. In this case, f has units of #/mg. f is determined during the simulation for each receptor location (node).

Empirical Model:
Using an empirically determined constant (b) that gives the ratio of contaminant concentration in air and in water (Pandis and Davidson 1999), inhalation dose (in mg or number of cells [#]) for one shower event can be estimated using the following equation:

$$D = bBC_wT_s \tag{4}$$

where B is the breathing rate (m^3/min), C_w is the contaminant concentration in water (mg/L or #/L), T_s is the duration of the shower (min), and the ratio b has units of L/m^3. This empirical model is available for use in TEVA-SPOT.

This approach assumes that equilibrium conditions exists throughout the duration of the shower and that transient effects related to turning the shower on and off can be neglected. Inhalation dose after the shower is turned off is assumed to be zero. If this approach is based on an equilibrium air concentration that is the same as the equilibrium air concentration predicted by the mass-balance approach, it will overestimate the inhalation dose relative to that estimated by the mass balance approach because it assumes that the contaminant air concentration is at the equilibrium value during the period immediately after the shower is turned on, when air concentration is actually smaller than the equilibrium value. For short duration showering events, equilibrium conditions may not occur during most of the event, if at all.

The ratio of the estimated dose obtained using the empirical approach to the estimated dose obtained using the mass-balance approach (with $T_2 = 0$) is shown in Fig. 5, as a function of shower duration, for several values of the removal rate. For a shower of average duration, the empirical approach yields estimated doses that are about 2 to 3 times larger than those obtained by the mass-balance approach, for values of the removal rate in the range of about 0.1 to 0.3 min^{-1}. The dose estimated by the empirical method approaches that estimated by the mass-balance method for long shower durations. Values for *b* are not contaminant specific. However, very few values for *b* have been published.

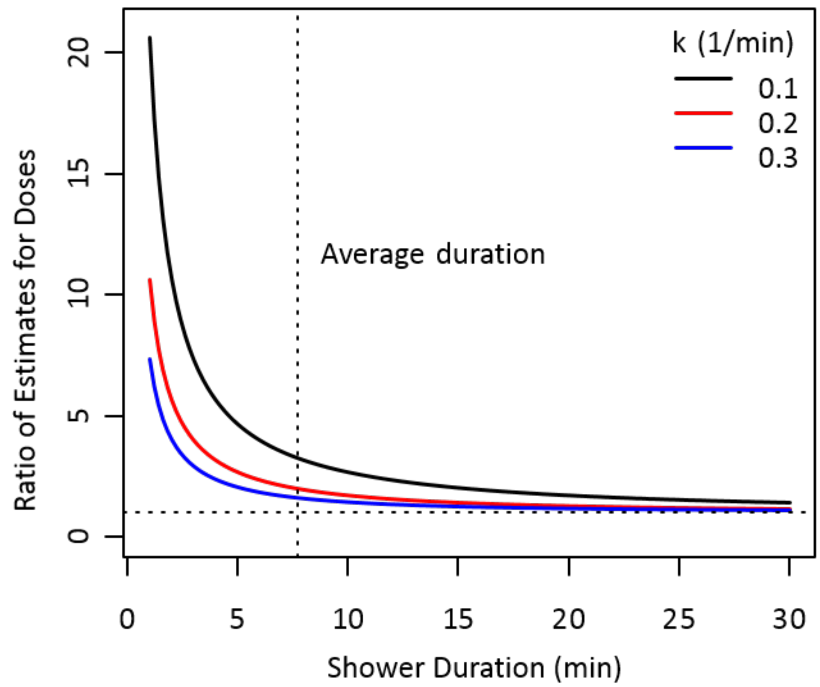

Figure 5: Ratio of Shower-Related Inhalation Doses for Contaminated Aerosols Estimated by the Empirical and Mass-Balance Approaches. It is assumed that equilibrium air concentrations are the same for both methods and $T_2 = 0$. k is the removal rate (air-exchange rate plus loss rate). The vertical dotted line indicates the average duration for a shower. A ratio equal to one is shown by the horizontal dotted line.

2.5.2 Volatilization

For volatile contaminants, inhalation dose is also determined using a model based on transient mass balance. Again, the model assumes complete, immediate mixing in the shower. Two approaches are presented here, one relying on the use of mass-transfer coefficients and the other using an average transfer efficiency for the removal of the contaminant from the shower water. Both of these approaches are available in TEVA-SPOT.

Mass-Transfer-Coefficient Model:
Concentration of the contaminant in shower air was determined following an approach outlined in Little and Chiu (1999). This concentration was then integrated over the duration of the shower to obtain an inhalation dose.

The flow of water through the shower is assumed to be simple plug flow: velocity is constant across the flow at any location from the shower head to the floor of the shower. The perimeter of the stream of water is constant.

To simplify the expression for inhalation dose, s_1 (units are mg/min/m^3) and r (units are min^{-1}) are defined as follows:

$$s_1 = \frac{QC_0}{V_s}(1 - exp(-K_{OL}A/Q)) \tag{5}$$

$$r = \frac{Q}{1000HV_s}(1 - exp(-K_{OL}A/Q)) + k_{on} \tag{6}$$

where Q is the water flow rate for the shower (L/min), C_0 is the water concentration of the contaminant when it enters the shower (mg/L), V_s is the volume of the shower stall (m^3), K_{OL} is the overall mass-transfer coefficient (L/min/m^2) based on the liquid-phase concentration, A is the interfacial area (m^2) that the mass transfer flux passes through, H is Henry's Law constant (dimensionless) for the contaminant[2], and k_{on} is the air exchange rate for the shower (min^{-1}) when it is on.

Using these definitions, and letting k_{off} be the air exchange rate for the shower when it is turned off, the inhalation dose, D, (in mg) for volatiles for one showering event is given by the following:

$$D = \frac{Bs_1}{r}[T_s - \frac{1}{r}(1 - exp(-rT_s)) + \frac{1}{k_{off}}(1 - exp(-rT_s))\,(1 - exp(-k_{off}T_2))] \tag{7}$$

where, again, B is the breathing rate (m^3/min), T_s is the duration of the shower (min), and T_2 is the time an individual remains in the shower stall after the shower is turned off (min).

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[2] The factor of 1000 (units L/m^3) is present because water concentration is in mg/L and air concentration is in mg/m^3. H is the ratio of equilibrium gas-phase and aqueous-phase concentrations of the contaminant. Henry's law constants depend on temperature and are generally given for a reference temperature (298.15 K or 25 °C). The user can provide a value for H for the reference temperature or provide a temperature-adjusted value, considering the temperature of the shower water.

If $T_2 = 0$, Eq. 7 reduces to the following:

$$D = \frac{Bs_1}{r}[T_s - \frac{1}{r}(1 - exp(-rT_s))] \quad (8)$$

Transfer-Efficiency Model:
Mass-transfer coefficients may not always be available and transfer efficiencies have been measured in some studies. The transfer efficiency is the weight fraction of the contaminant that is volatilized from the shower water. Air concentration of contaminant was determined following the method used by Xu and Weisel (2003) and integrated over the duration of the shower to obtain an inhalation dose. Using a transfer efficiency, the inhalation dose (mg) for volatiles for one shower event is given by the following:

$$D = \frac{Bs_2}{k_{on}}\left[T_s - \frac{1}{k_{on}}(1 - \exp(-k_{on}T_s)) + \frac{1}{k_{off}}(1 - \exp(-k_{on}T_s))\,(1 - \exp(-k_{off}\mathrm{T}_2))\right] \quad (9)$$

where $s_2 = QT_eC_0/V_s$ and T_e is the average transfer efficiency for removal of volatile chemicals from shower water. T_e can vary from 0 to 1. If $T_2 = 0$, Eq. 9 reduces to the following:

$$D = \frac{Bs_2}{k_{on}}[T_s - \frac{1}{k_{on}}(1 - exp(-k_{on}T_s)) \quad (10)$$

2.5.3 Discussion

Table 2 summarizes the parameters that a user needs to provide to use the various approaches for estimating inhalation dose. The table also provides default values for most parameters. The user also needs to specify the bins to be used to report results for inhalation dose. If health-effect end points (e.g., fatalities) are needed, the user must specify the appropriate dose- response information.

The default value for breathing rate provided in the table is the mean value for most age groups given in Table 6-2 of EPA's Exposure Factors Handbook (U.S. EPA 2011) for light intensity activity. The value is the recommended short-term exposure value for males and females combined.

For all the models used for estimating doses, dose is proportional to the contaminant concentration in the water feeding the shower. Consequently, doses can be estimated for unit concentrations of a contaminant for each receptor before beginning a simulation and these doses can then simply be multiplied by water concentrations determined during the simulation for each showering event.

Table 2. Parameters Required for Estimating Doses for Showering

Process	Model	User-provided parameters[a]	Default values
Aerosolization	Mass balance (Eq. 1)	B	0.012 m^3/min
		G	6.0 mg/min
		V_s	2 m^3
		k_1	0.3 min^{-1}
		k_2	0.1 min^{-1}
		T_2	0
	Empirical (Eq. 4)	b	No default
		B	0.012 m^3/min
Volatilization	Mass transfer coeff. (Eq. 7)	B	0.012 m^3/min
		Q	9 L/min
		V_s	2 m^3
		H	–b
		$K_{OL}A$	–b
		kon	0.15 min^{-1}
		$koff$	0.075 min^{-1}
		T_2	0
	Transfer efficiency (Eq. 9)	B	0.012 m^3/min
		Q	9 L/min
		T_e	0.8
		V_s	2 m^3
		kon	0.15 min^{-1}
		$koff$	0.075 min^{-1}
		T_2	0

[a]Parameters are defined in the text. [b]These parameters are contaminant specific.

3 Humidifier Use

3.1 Introduction

The approach for estimating inhalation doses associated with the use of an ultrasonic or cool-mist humidifier is essentially the same as that used for estimating inhalation doses associated with showering. The only differences are that the values of the parameters are different and transient effects are neglected. These humidifiers are very efficient generators of aerosol particles. Therefore, even though the rate at which water is used in a humidifier is much less than that in a shower, the rate at which aerosols are generated can be larger. Because of the relatively small volume of water used in a humidifier, they are less important as a source of volatile contaminants than a shower, which can remove a sizeable fraction of volatile contaminants from a much larger volume of water.

Unfortunately, relatively little information appears to be available on humidifier use. Consequently, an approach to estimating inhalation doses that is suitable for performing sensitivity analyses is needed. This section describes the capability added to TEVA-SPOT for carrying out such analyses.

Relative to showering, the duration of exposures to contaminants released by a humidifier can be very long. The average duration of a shower is less than eight minutes. Exposures related to a humidifier can last eight hours or more. Consequently, the transient effects associated with turning on and turning off a humidifier are less important than such effects are for a shower. The approach presented here for humidifiers is based on the assumption that contaminant air concentration is constant and at its equilibrium value throughout the entire exposure period. Turn-on and turn-off periods are neglected.

Estimating inhalation doses for humidifiers requires information on three different topics: (1) the behavior of the user of the humidifier, (2) the characteristics of the humidifier, and (3) the environment in which the humidifier is used. Information on the last two topics is available. Limited information is available for user behavior.

This section outlines how inhalation doses can be determined for a single use of a humidifier (a humidifier event) that has been filled with contaminated water from a distribution system. Humidifiers are assumed to be filled daily immediately before they are operated. Individuals who used humidifiers are assumed to use them every day during the course of a simulation. The only difference between the daily events for an individual is that contaminant concentration in the water used to fill the humidifier will generally change. Total inhalation dose for a receptor for a simulation is determined by summing the doses for the separate, daily events. Results for individual receptors are combined for each scenario to obtain impacts by dose level as is done for ingestion dose. The user needs to specify the dose bins to use to reports impacts by scenario. The various parameters needed to estimate inhalation doses are discussed in Section 3.2 and the approaches used to estimate dose are given in Section 3.3.

3.2 Parameters

3.2.1 Behavior

Several parameters need to be quantified to describe behavior: (1) What fraction of the population uses a humidifier, (2) When is water added to the humidifier, and (3) How long is the humidifier used. Good information is not available on these parameters.

The fraction of the population that uses a humidifier can vary from 0.0 to 1.0. All individuals using water from the network are potential users of humidifiers and use is assigned randomly to the fraction of the population specified. The default value is 0.2. Limited information is available on the fraction of the population that uses a humidifier. TEVA-SPOT allows the user to easily vary this and other parameters in order to perform sensitivity analyses.

Receptors are assumed to be exposed to contaminants released by a humidifier for some duration of time specified by the user. The default assumption is that the humidifier is used while sleeping and the duration of exposure is eight hours.

No data are likely to be available on when humidifiers are filled with water. In order to determine contaminant concentration in the fill water, a time must be specified. The default assumption is that humidifiers are filled immediately before use and that this occurs at 22:00 hours.

Behavior is assumed to be the same for every day in a simulation. Only one event involving humidifier use is assumed to occur in a day.

Although not strictly a parameter related to behavior, a breathing rate for receptors is needed. This rate needs to be consistent with the assumed use of the humidifier. If the humidifier is used while sleeping, then the appropriate breathing rate is the average short-term rate for adults while sleeping. This value is 0.3 m^3/h, which is the default value. Values for breathing rates are provided in Table 6-2 of U.S. EPA (2011).

3.2.2 Humidifier Description

The humidifier is assumed to convert all water in the humidifier into inhalable aerosol particles. The only parameter needed to describe the humidifier is the rate at which water is used. The default rate is 0.5 L/h.

3.2.3 Environment

The only parameters needed to describe the environment are the volume of the room in which the humidifier and the receptor are located and the total loss rate for the aerosols. The default values are 30 m^3 (1,060 ft^3) and 1.0 h^{-1}, respectively.

3.3 Estimating Doses

Two approaches are available in TEVA-SPOT for estimating inhalation doses resulting from exposure to contaminated aerosols generated by a humidifier. The first approach is based on mass balance and requires the user to specify the water use rate for the humidifier and the removal rate for aerosols. The second approach uses a purely empirical constant to relate contaminant concentration in the air to contaminant concentration in the water used in the humidifier. As is the case for inhalation doses estimated for showering, the estimated doses associated with humidifier use are also potential inhalation doses and equal the mass of contaminant that enters the body by inhalation.

3.3.1 Mass-Balance Model

The mass-balance model assumes complete mixing of the contaminant in the air of the room and neglects transient effects. The inhalation dose, *D* (mg or number of cells) for one humidifier event is shown in Eq. 11:

$$D = \frac{BGC_w T_h}{kV} \tag{11}$$

where B is the breathing rate (m^3/h), G is the aerosol volume generation rate (L/h), C_w is the contaminant concentration in the humidifier water (mg/L or #/L), T_h is the duration of exposure (h), k is the removal rate for aerosols (h^{-1}), and V is the volume of the room (m^3). The removal rate is the sum of the air exchange rate for the room and the loss rate for the aerosols.

The aerosol generation rate equals the water use rate. All water is assumed to be converted into inhalable aerosols and released into the room, which is a conservative assumption. The contaminant concentration in the water equals the contaminant concentration in the water in the distribution system at the location of the receptor at the time the water is withdrawn for use in the humidifier.

3.3.2 Empirical Model

Using an empirically determined constant (b) that gives the ratio of contaminant concentration in air and in water, inhalation dose (in mg or number of cells) for one humidifier event can be estimated using the following equation:

$$D = bBC_wT_h \tag{12}$$

where the ratio b has units of L/m^3.

3.4 Summary

The various parameters that a user needs to be specify when estimating humidifier related doses and their default values are summarized in Table 3. The user also needs to specify the bins to be used to report numbers of individuals with inhalation doses greater than the threshold values specified for the bins. Additionally, the user can specify the dose-response information needed to determine associated health-effect end points.

4 Additional Calculations

Sections 2 and 3 present approaches for estimating inhalation doses associated with showering or humidifier use. This section discusses options for (1) presenting results in terms of exposure duration and air concentration of contaminant rather than dose and (2) providing results that can be used to evaluate the relative importance of the major exposure event associated with either showering or humidifier use that an individual experiences during a contamination event. An individual may experience multiple exposure events during the period in which a WDS is contaminated.

Table 3. Parameters Required for Estimating Doses for Humidifiers

Model	User-provided parameters[a]	Default value
Mass balance	B	0.3 m^3/h
(Eq. 11)	G	0.5 L/h
	V	30 m^3
	k	1.0 h^{-1}
	T_h	8 h
Empirical	b	No default value
(Eq. 12)	B	0.3 m^3/h
	T_h	8 h
Both	Fraction of population using a humidifier	0.2
	Time water is added	22:00 hours

[a]The user-provided parameters in this column are defined in the text.

For some contaminants there is a preference for using contaminant concentration (C) and exposure duration (T) rather than dose as the metric of interest. Two options are available in TEVA-SPOT that allow the user to examine consequences in this alternative way. The approaches used in these options are based on the assumption that the great majority of an individual's dose is accumulated during one exposure event. This may not be a good assumption; however, the dose estimates available to the user give only cumulative values, so the user cannot be certain about the validity of the assumption. Therefore, an additional option is included that allows the user to examine the degree to which cumulative dose is the result of one or more exposure events.

4.1 Reporting Results for C×T

For the case in which inhalation dose is the result of a single exposure event of duration T (min) with a constant air concentration of C (mg/m^3) for an individual with a breathing rate B (m^3/min), the dose (mg) is given by:

$$D = BCT \tag{13}$$

Therefore, if D is known, C×T is simply D/B. Note that for showering, $T = T_s + T_2$. Generally, values of C×T are of interest only for some chemical contaminants.

Assuming that the doses determined by the various approaches given in Section 2.5 or Section 3.3 are the result of a single exposure event (or at least a series of events in which one is dominant), an estimate for C×T for the dominant event can be determined for each receptor by dividing the cumulative dose calculated for the receptor by the breathing rate. This is done by TEVA-SPOT in parallel with dose calculations, with a separate binning of C×T values. The user needs to specify the bins to be used. Alternatively, if no dose calculations are being done, values for C×T can be obtained by simply performing the dose calculations with a value of B = 1. The approach outlined here gives the product of the sum of the average concentrations for each of the exposure events for an individual multiplied by the event duration (which is the same for all events of the same type for a given receptor). If exposure to the contaminant occurs during only one exposure event, then this approach gives the product of the average air concentration of the contaminant for that event times the duration of the event.

4.2 Reporting Separate Results for C and T

For some contaminants, the health effects resulting from exposure to the contaminant are the same, or approximately the same, for different events if the product C×T remains the same, even if the values for C and T vary from event to event. In other words, the consequences do not depend on dose rate. This has been the implicit assumption in all calculations involving multiple exposures spread over a long simulation. However, for some contaminants the values of C and T, and not just their product, are important. Therefore, TEVA-SPOT allows reporting of results for both C and T and not just their product or dose.

If values for C and T are to be reported, these values should be for the major event for a receptor during the simulation. The major event is the one for which the water concentration of the contaminant is largest. Therefore, for each receptor for the event with the maximum water concentration the exposure duration ($T_s + T_2$ for showering and T_h for humidifier use) and the average air concentration in the shower stall or the room in which a humidifier is used is retained and then binned for the scenario. The average air concentration equals $\frac{D}{BT}$ for the event. The binning is two dimensional because the two quantities C and T are needed. The results are the number of receptors with values of C and T who are in each bin. The user needs to specify the bins for both C and T.

4.3 Examination of Importance of Individual Exposure Events

The results obtained using the preceding two options are only useful if the great majority of inhalation dose is accumulated during a single exposure event. This option provides the ability to determine if this is a good assumption for a particular evaluation for a network.

As noted above, the event of most importance for each individual is the one with the largest water concentration of the contaminant. The relative contribution of this event is the dose estimated for the event divided by the total dose determined for the individual for the entire simulation. For each individual who showers or uses a humidifier and who accumulates an inhalation dose greater than zero the relative contribution of the major event is determined. Its value will always be less than or equal to one. These values are binned for all individuals for each scenario using 10 equally spaced bins extending from 0 to 1.0. The binned results are reported for the scenario and also combined to yield binned results for the entire ensemble.

Many receptors will receive little or no dose and are of no particular importance for these calculations. The user needs to specify multiple thresholds for dose above which binned relative-importance values are to be reported. For example, if the dose threshold specified is 1.0 mg, the results will be, for each of the scenarios evaluated and for the ensemble of scenarios, the numbers of individuals receiving an inhalation dose of this size or greater whose relative-importance values for the major exposure event are in each of the 10 bins that extend from 0 to 1.0. Using a number of dose thresholds it is possible to determine if the relative importance of major exposure events changes as the dose threshold changes.

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