

APPENDIX C

STEADY-STATE MODE

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STEADY-STATE MODE

TRIM.FaTE can be run in two modes: dynamic or steady-state. This appendix describes implementation of the TRIM.FaTE steady-state mode (Section C.1) and potential user applications of that feature (Section C.2). The advantage of the steady-state mode is that the run time is very short compared with typical dynamic runs that use hourly-to-daily simulation time steps over the course of many years (*e.g.*, 30-year). The short run-time allows the user to quickly test new approaches and to conduct sensitivity or Monte Carlo analyses that would be require much greater run times if the dynamic mode were used.

C.1 STEADY-STATE SOLUTION FEATURE

The description of TRIM.FaTE in Chapters 1 through 8 apply to both dynamic and steady-state modes except where noted below. The remainder of this section describes important differences between the steady-state and dynamic modes.

Section C.1.1 describes how to develop constant values for time-varying model inputs. Section C.1.2 describes changing the air transfer factors in the dynamic mode to implement the steady-state mode. Section C.1.3 notes changes that are needed with respect to the ground-water transfer factors. Finally, Section C.1.4 describes other differences in the TRIM.FaTE code setup for the steady-state versus dynamic modes.

C.1.1 CHANGING TIME-VARYING INPUT DATA TO CONSTANTS

Generating steady-state results with the model requires representative steady-state values for the time-varying inputs in the current version of the TRIM.FaTE library. The primary time-varying inputs include:

- wind speed;
- wind direction;
- mixing height;
- rain;
- *IsDay* (0 at night; = 1 during the day);
- *AllowExchange* (0 during non-growing season; = 1 during growing season);
- litter fall (*e.g.*, deciduous forest and grasses/herbs); and
- river flow.

Many of these time-varying inputs combine and interact to influence specific transfer factors within TRIM.FaTE, and the different time-varying inputs interact/combine in different ways when used in different algorithms. For example, wind speed and direction influence the relative magnitude of the advective air transfers along the interfaces between air compartments. Other transfer factors are influenced in a discontinuous fashion, as for example the transfer factors that include the variable I_{wet} , the proportion of the wet deposition of chemical sorbed to dust particles (or in vapor phase) that is intercepted and retained on the plants. The variable I_{wet} is a function of the leaf area index (*LAI*), mixing height, rain, and *AllowExchange*. When

AllowExchange is zero, the wet interception fraction is zero. Thus, it is not appropriate to simply assign an average value for each of the time varying inputs and assume that would result in appropriate values for the calculated transfer factors. In addition to providing representative values for the time-varying inputs, a number of calculated transfer factors need to be assigned steady-state values.

The calculated steady-state variables (or distributions) that need to be considered include:

- Advective transfers across each air-to-air interface including external boundaries of the system (calculated as function of wind speed, wind direction, mixing height, and parcel coordinates) (Section C.1.1.1);
- Dry interception fraction for vegetation (calculated as function of *AllowExchange*, mixing height, and the wet biomass of the vegetation per unit area) (Section C.1.1.2);
- Wet interception fraction (calculated as function of *AllowExchange*, rain, mixing height, and *LAI*) (Section C.1.1.3);
- Diffusive transfer across air/stomata interface (calculated as function of *LAI*, *IsDay*, and mixing height) and diffusive transfer across air/cuticle interface (calculated as function of *LAI* and mixing height) (Section C.1.1.4);
- Litter fall (*e.g.*, deciduous forest and grasses/herbs) and river flow (Section C.1.1.5); and
- Plant intake rates for wildlife, which are modified by the *AllowExchange* variable (Section C.1.1.6).

Steady-state models have typically used long-term arithmetic mean (*AM*) values for the inputs, but we are not aware of any research that has evaluated whether those *AM* inputs are more appropriate than other indications of central tendency (*e.g.*, median, geometric mean, etc.) for estimating steady-state output in a spatially segmented dynamic model. Fortunately, this problem should not affect a steady-state uncertainty or sensitivity analysis because the user is generally most interested in the *relative* propagation of uncertainty/variability through the model for a given set of inputs. To maintain consistency with the other TRIM.FaTE inputs, we recommend using the *AM* input values (and distributions) for the calculated time-varying inputs and for the transfer factors in the steady-state scenario. For hourly meteorological data, the *AM* value for each year of meteorological data can be calculated. The annual average values can then be used to estimate a long-term average, and an appropriate statistical model can be used to describe the set of annual average values.

C.1.1.1 Advective Air-to-air Transfers

A challenge that arises in calculating steady-state inputs for use in the advective air transfers is that the time-varying inputs from the meteorological data files per unit time are not normally distributed. As a result, the long-term average transfer factor estimated at the simulation time steps from the transfer factors may differ from that estimated from the long-term average inputs for a given mass-transfer process. We use an example to illustrate this challenge below.

In its simplest form, the advective transfer factor (/day) across an interface between two neighboring air parcels is given by:

$$T_{As \rightarrow Ar} = \frac{flux_{s \rightarrow r}}{V_s} \quad (\text{TF C-1})$$

where $flux_{s \rightarrow r}$ is the flux of air across the interface (m^3/d) from sending compartment s , to receiving compartment r , and V_s is the volume of the sending compartment. Assuming that the long-term arithmetic mean (AM) transfer factor is a good surrogate for steady state, we can calculate the $AM[T_{As \rightarrow Ar}]$ in two ways. The first way calculates a value of $T_{As \rightarrow Ar}$ for each hour of meteorological data and then estimates the long-term average transfer factor from this set of hourly values:

$$AM[T_{As \rightarrow Ar}] = \frac{1}{n} \times \sum_{j=1}^n T_{As \rightarrow Ar} \quad (\text{Eq. C-1})$$

where j represents the hour and n is the total number of hours (*i.e.*, $n = 8760$ for one year of meteorological data). The second way calculates the average values of $flux_{s \rightarrow r}$ and V_s from the set of hourly values for these variables, then estimates the steady state $T_{As \rightarrow Ar}$ as the quotient of the two average values such that:

$$AM[T_{As \rightarrow Ar}] = \frac{AM[f_{s \rightarrow r}]}{AM[V_s]} \quad (\text{Eq. C-2})$$

However, if the hourly values for flow and/or volume are not normally distributed (which they are not) then the two approaches give different answers:

$$\frac{1}{n} \times \sum_{j=1}^n T_{As \rightarrow Ar} \neq \frac{AM[f_{s \rightarrow r}]}{AM[V_s]} \quad (\text{Eq. C-3})$$

In other words, the arithmetic mean (AM) of the set of hourly transfer factors does not equal the quotient of the $AM [flux_{s \rightarrow r}]$ and the $AM [V_s]$.

To illustrate the difference, we use the first year's hourly meteorological data prepared for the mercury test case to calculate advective transfer across one of the segments of the parcel that included the source facility. The $AM[T_{As \rightarrow Ar}]$ calculated from the 8760 hourly transfer factors

(excluding the zeros) was 19.9 /hr. The transfer factor calculated from the quotient of average flow and volume was 12.7 /hr, a difference of about 40 percent.

The steady-state input for transfer across an air-to-air interface is dependent on wind speed, wind direction, mixing height, and the coordinates of the interface (length and angle). In addition, the actual transfer also depends on the volume of the sending compartment, which in turn depends on the atmospheric mixing height. In the mercury test case, we actually calculated the transfer factor for each interface using both of the methods described earlier (*i.e.*, Equations C-1 and C-2).

For Eq. C-2, the value of $T_{As \rightarrow Ar}^j$ for the j^{th} hour of the meteorological data is given by:

$$T_{As \rightarrow Ar}^j = \frac{u}{\sqrt{(y_2 - y_1)^2 + (x_2 - x_1)^2}} \times [(y_2 - y_1) \sin \vartheta - (x_2 - x_1) \cos \vartheta] \times \frac{A_i}{V_{sj}} \quad (\text{TF C-2})$$

where u is the wind speed (m/day) towards the direction ϑ across the compartment boundary during the j^{th} hour, A_i is the area of the interface given by the time-varying mixing height h_j (m), and length of compartment interface, L_i (m). The volume of the sending compartment, V_{sj} , is also a function of the time-varying mixing height. The L_i is constant over time and is defined by two Cartesian coordinates ($P_1 = (x_1, y_1)$, $P_2 = (x_2, y_2)$) where the coordinates of each segment of a polygon are evaluated in clockwise order and the length is:

$$L_i = \sqrt{(y_2 - y_1)^2 + (x_2 - x_1)^2} \quad (\text{Eq. C-4})$$

TF C-2 can be simplified for each hourly time step to give the following transfer-factor algorithm:

$$T_{As \rightarrow Ar}^j = \frac{u}{A_i} [(y_2 - y_1) \sin \vartheta - (x_2 - x_1) \cos \vartheta] \quad (\text{TF-C-3})$$

Evaluating the coordinates in clockwise order around a given polygon results in a negative value for transfer out of the polygon and a positive value for transfer into the polygon (wind direction is also reported as degrees clockwise from North). In estimating steady-state transfer factors, the user is only interested in transfers out of a given polygon across a given interface. Thus, the positive values can be ignored and the absolute values of transfers out of the polygon (*i.e.*, from the sending compartment) are used. In the example for the mercury test case, we calculated values of $AM[T_{As \rightarrow Ar}^j]$ for each of the five years of meteorological data, which resulted in a distribution of $AM[T_{As \rightarrow Ar}^j]$ values for each line segment and direction.

We also calculated the transfer factor for each year by summing the annual volumetric flux across the interface and using the long-term average mixing height and constant area of the

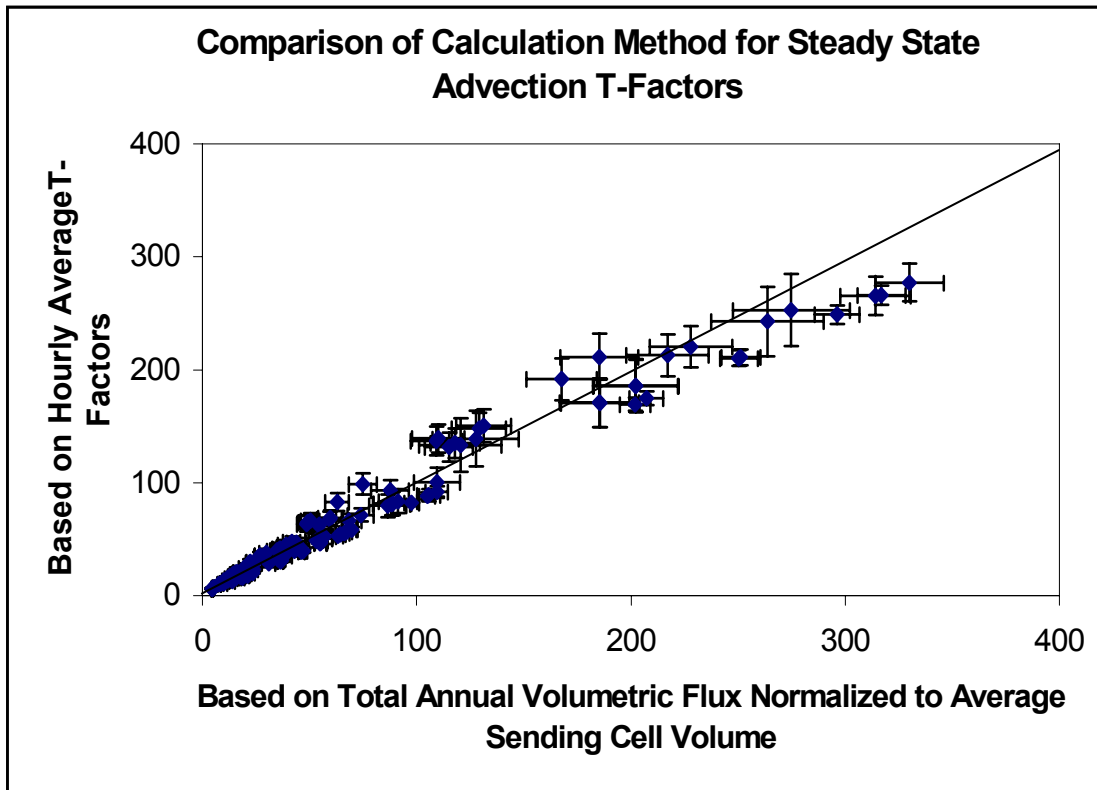


Figure C-1. Comparison of long-term average advective transfer factors calculated using the daily average volumetric flux normalized to sending compartment (cell) volume (x-axis) and the average of the hourly transfer factors (y-axis).

sending compartment to estimate the transfer factor using Eq. C-2. The difference between the two methods is illustrated in Figure C-1. The overall difference in the results of the two methods was not great. (In the mercury test case, we combined the two sets of results to provide a single estimate of the transfer factor for each interface).

It is important to remember that the steady-state value (or distribution) for a given transfer factor represents a long-term average transfer, not day-to-day or hour-to-hour variation in the transfer.

C.1.1.2 Dry Interception Fraction

For deciduous plants and grasses/herbs, the dry interception fraction is a function of *AllowExchange*, mixing height, and biomass (wet wt) of the vegetation per unit area. For coniferous plants that do not lose their leaves seasonally, the dry interception fraction is assumed to be a constant value throughout the year.

The dry interception fraction, I_{dry} , is calculated for deciduous plants and grasses/herbs as receiving compartments per Eq. 7-2 of TSD Volume II, as modified to accommodate a steady-state *AllowExchange* variable:

$$I_{dry} = 1 - \exp\left[\left(1 - fW_{Leaf}\right)\left(-\alpha_{VAF} \times AllowExchange \times \rho_{area}\right)\right] \quad (\text{Eq. C-5})$$

where, for both grasses/herbs and deciduous plants, fW_{Leaf} is the water content of the plant (0.8, unitless), α_{VAF} is the vegetation attenuation factor (-2.9 m²[leaf]/kg[plant dry wt]), and ρ_{area} is the areal density of above-ground non-woody vegetation (0.6 kg[plant wet wt]/m²[surface soil]). *AllowExchange* is used as a seasonal on/off switch for the interception fraction. When *AllowExchange* is one, I_{dry} is calculated by Eq. C-5, but when *AllowExchange* is zero, I_{dry} is zero.

The volume of the sending air compartment, V_s , is also used to calculate the transfer factor for dry deposition (see TF 7-1 in TSD Volume II). Due to hourly changes in the mixing height, the long-term average V_s can differ during times when *AllowExchange* is on and when it is off, as illustrated in Figure C-2. Therefore, the steady-state value of I_{dry} needs to be normalized to a sending compartment volume that is relevant to the time when leaves are intercepting particles (*i.e.*, when *AllowExchange* = 1). The factor used to normalize the steady-state interception fraction is the long-term (annual) average mixing height divided by the average mixing height when *AllowExchange* is equal to 1. In summary, the steady-state I_{dry} value for each of the five years is given by:

$$SS.I_{dry,j} = \frac{\bar{h}(AE = 1,0)}{\bar{h}(AE = 1)} \times \frac{1}{n} \times \sum_{j=1}^n I_{dry,j} \quad (\text{Eq. C-6})$$

where $h(AE=1,0)$ represents the average over the full year and $h(AE=1)$ represents average mixing height when *AllowExchange* is set to 1.

C.1.1.3 Wet Interception Fraction

The wet interception fraction, I_{wet} , is a function of total rain for each rain event, the seasonal LAI (calculated from the average leaf area interface and the *AllowExchange* variable) and, as with the dry interception fraction, a normalization factor to the appropriate average air mixing height. Wet interception is calculated by Equation 7-4 of the TSD Volume II as modified to accommodate the *AllowExchange* variable and the cumulative rain for a given rainfall event. We define a rainfall event as the cumulative time over which rain occurs, which is bracketed (before and after) by at least one hour with no rain. Given this definition of *rain*, the wet interception fraction for rain event k is:

$$I_{wet,k} = \frac{AllowExchange \times LAI \times S}{rain} \times \left[1 - \exp\left(\frac{-\ln(2)}{3 \times S} \times rain\right)\right] \quad (\text{Eq. C-7})$$

Distribution of Mixing Height

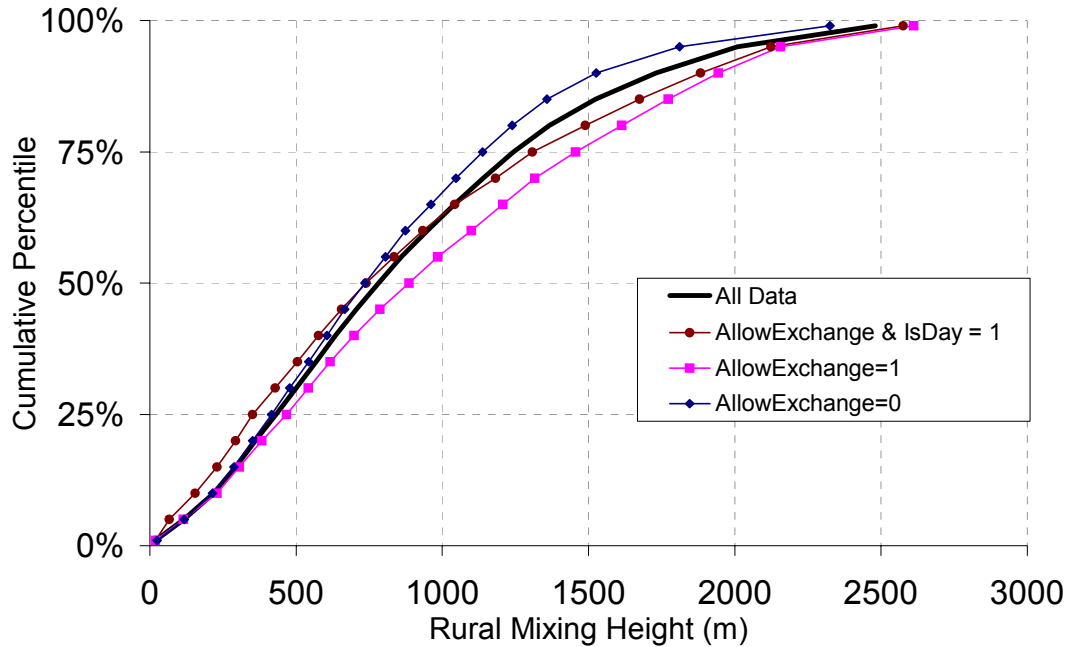


Figure C-2: Distributions of hourly mixing height reported for different conditions where *AllowExchange* controls seasonality and *IsDay* is used in the model to modify stomata diffusion.

where k indicates the k^{th} rain event, S is the leaf wetting factor (0.0003 m) and LAI is the leaf area index (grasses/herbs = 5, deciduous forest = 3.4 and coniferous forest = 5). The I_{wet} for the k^{th} event is multiplied by the cumulative amount of rain for that event to give the volume of intercepted rain. The event-specific volume of intercepted rain is summed over the year to give the total volume of “intercepted” rain. The long-term interception fraction is then estimated as the intercepted volume for the given year divided by the cumulative rain for that year.

As with I_{dry} , the final steady-state value for wet interception (for each year) is normalized to account for differences between the overall average mixing height of the sending compartment and the average mixing height when it is both raining and the *AllowExchange* variable is 1 such that:

$$SS.I_{wet} = \frac{\bar{h}(AE = 1,0)}{\bar{h}(AE = 1 \& rain > 0)} \times \frac{1}{n} \times \sum_{j=1}^n I_{wet,j} \quad (\text{Eq. C-8})$$

where $AE=1 \& rain > 0$ indicates that both the *AllowExchange* variable = 1 and it is raining.

C.1.1.4 Diffusive Transfer Across Air/Stomata Interface and Across Air/Cuticle Interface

This diffusive transfer combines two process where the stomata transfer is controlled by the *LAI (AllowExchange)*, *IsDay*, and the relative mixing height during exchange (*i.e.*, when *LAI* and *IsDay* are both 1) and where the cuticle transfer is influenced only by *LAI (AllowExchange)* and relative mixing height. The two parts of the equation need to be treated separately so that each mass transfer process can be independently modified by either the *AllowExchange* variable (cuticle) or the combined *AllowExchange.IsDay* variable (stomata).

The first *AllowExchange* variable, the one that modifies cuticle exchange, is the same height-normalized value that is used for I_{dry} . In this case, we derive a single steady-state value for *AllowExchange* that modifies both I_{dry} and the cuticle side of the air-to-plant diffusion equation.

The steady-state modification factor for the stomata diffusion is calculated as the long-term average of the product of *IsDay*, input as a fraction representing the average number of daylight hours per 24-hr period, and *AllowExchange*, adjusted for height of the sending compartment, using the following normalization factor:

$$NormalizationFactor = \frac{\bar{h}(AE = 1, 0)}{\bar{h}(AE = 1 \& ID = 1)} \quad (\text{Eq. C-9})$$

where $AE=1 \& ID=1$ indicates that both *AllowExchange* and *IsDay* are equal to one.

These two steady-state modification factors are incorporated into the equation for total diffusive transfer across the air/plant interface so that both the stomata pathway and the cuticle pathway are transformed to steady state.

C.1.1.5 Litter Fall and River Flow

In the current TRIM.FaTE library, the litter-fall rate constant, k_L , for deciduous forests and for grasses/herbs is set such that 99 percent of the mass is transferred to soil in approximately one month.¹ To run TRIM.FaTE in the steady-state mode, this litter-fall rate is transformed such that 99 percent of the mass is transferred to soil on an annual basis (365 days):

$$0.01 = \exp(-k_L \times 365) \quad (\text{Eq. C-10})$$

Solving Equation C-10 for k_L gives a steady-state litter-fall rate constant of 0.013 /day. The litter-fall rate for coniferous plants does not change from the rate used for TRIM.FaTE in the dynamic mode. The user can set a date for harvest of agricultural plants or allow them to become litter.

¹In the current TRIM.FaTE library, the litter-fall rate constant for coniferous forest is set to a value that is constant throughout the year. For the agricultural plants, the user can set the date of harvest, and the chemical mass in the harvested biomass can be transferred to a sink.

The steady-state flow of a river is simply the time-weighted average flow (or velocity).

C.1.1.6 Wildlife Plant Ingestion Rates

The wildlife plant ingestion rates (i.e., total ingestion rate \times fraction of diet that consists of plants on a wet weight basis) are multiplied by *AllowExchange* to ensure that wildlife only consume plant leaves during the growing season. For a steady-state run, *AllowExchange* is set to a fractional value equal to the number of days it is equal to 1 divided by 365 days per year to get an annual average.

C.1.2 SWITCHING ADVECTIVE AIR TRANSPORT ALGORITHMS

Switching from the dynamic to the steady-state advective air transport algorithms involves three steps:

- (1) Enabling the steady-state algorithms;
- (2) Disabling the dynamic algorithms; and
- (3) Setting up the steady-state advective transfer factors.

The steady-state air advective transfer factors are used to calculate air advection (see Section C.1.1.1). Two transfer factors (two directions) are calculated for each interface between one air volume element and an adjacent air volume element. In addition, the user should calculate transfer factors across each interface from air volume elements bounding the exterior of the modeling domain to the air sinks (i.e., moving chemical mass from the boundary air volume elements into the air sinks). These transfer factors can be calculated by hand (in a spreadsheet) using the meteorological data set and information about the spatial relationships of the air volume elements. The number of years of meteorological data to average for each interface depends on the number of years associated with any apparent cycle or pattern of meteorologic conditions that is repeated at intervals (e.g., five years in the mercury test case). The steady-state air advective transfer factors are simply set equal to the calculated value for a particular link.

The use of the steady-state air advection transfer factors for each air/air compartment interface results in a more accurate representation of the average advective flows between air compartments than simply using average values for all of the meteorological properties and allowing the model to use those values in the existing dynamic air advection transfer algorithms. The use of steady-state air advection transfer factors (see Section C.1.1) retains information on correlations among the meteorological properties (e.g., a certain wind direction may be associated with higher wind speeds) that would be lost in an overall averaging process.

At the moment, the steady-state air advection transfer factors for each air/air compartment interface must be calculated outside of TRIM.FaTE (e.g., using spreadsheets). We expect that future versions of TRIM.FaTE will include the ability to calculate these transfer factors internally, thus reducing the time required of the user to set up a steady-state simulation.

C.1.3 DISABLING LINKS WITH GROUND WATER

A limitation of applying the steady-state mode is the inability to accommodate ground water. Thus, the final step in setting up a steady-state simulation is disabling all of the links from groundwater to other compartments (*i.e.*, vadose-zone soil and surface water). This step is required because the groundwater compartments lose mass so slowly that the steady-state solver cannot find a solution. After disabling the dynamic-mode links to and from groundwater, the ground-water compartment basically acts as a sink for chemical mass. Then, the steady-state solver is able to calculate a solution.

C.2 APPLICATIONS OF THE STEADY-STATE MODE

The speed of the steady-state solution makes it attractive for several types of applications (*e.g.*, diagnostic and uncertainty analyses).

As a diagnostic tool, the steady-state mode, with its short run time, can be used in evaluating the impact of changes to the set-up of a simulation, as well as parameter values and algorithms. The ability to perform a large number of realizations in reasonable run time (as provided in the steady-state mode) gives the user the opportunity to investigate model behavior. If the results from TRIM.FaTE appear inconsistent with expectations or with existing data, the user can quickly test different hypotheses about how those results were produced. During this exercise, the user can modify certain input parameters or assess different formulas for transfer factor algorithms (or for various compartment properties) and quickly assess the response of the model results to those changes.

In uncertainty and sensitivity analyses, the steady-state mode is also a valuable tool. For large and/or complex parcel layouts, sensitivity analyses of the many property values in a simulation when run in dynamic mode (*e.g.*, involving simulations of many years) can involve substantial run times. Similarly, dynamic simulations involving Monte Carlo assignment of key property values can also be time consuming. The steady-state mode can be used to provide a Monte Carlo sampling-based sensitivity analysis of many properties in a reasonable run time. This enables examination of the sensitivity of the model results to a much larger number of variables than would be possible using the sensitivity analysis feature in the dynamic mode in the same amount of run time.

Information from sensitivity/Monte Carlo analyses conducted using the steady-state mode can then be used to select a small number of input parameters for which the user can run a dynamic-mode uncertainty analysis. The final uncertainty analysis could then be a set of fully dynamic runs that produce a family of time-series curves (or an uncertainty band around an outcome curve). Results from the steady-state uncertainty/sensitivity analysis might also be evaluated as to their use to predict the outcome variance in the dynamic runs.

Appendix D

TABLES OF TRIM.FaTE INPUT PARAMETERS

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