6. TREATMENT OF UNCERTAINTY AND VARIABILITY

This chapter summarizes the approach for assessing uncertainty and variability in TRIM.FaTE, which follows the general approach for TRIM as described in Chapter 3 of the TRIM Status Report (USEPA 1999). Additional background on how this method was selected is provided in Appendix B of the TRIM Status Report (USEPA 1999). The following text box presents definitions for the key terms used in this chapter to explain the uncertainty and variability analysis framework for TRIM.FaTE.

KEY TERMS FOR UNCERTAINTY AND VARIABILITY ANALYSIS

Variability

Variability represents the diversity or heterogeneity in a population or parameter, and is sometimes referred to as natural variability. An example is the variation in the heights of people. Variability cannot be reduced by using more measurements or measurements with increased precision (*e.g.*, taking more precise measurements of people's heights does not reduce the natural variation in heights). However, it can often be accounted for by a more detailed model formulation (*e.g.*, modeling peoples' heights in terms of age will reduce the unexplained variability due to variation of heights).

Uncertainty

Uncertainty refers to the lack of knowledge regarding the actual values of model input variables (parameter uncertainty) and of physical systems (model uncertainty). For example, parameter uncertainty results when non-representative sampling (to measure the distribution of parameter values) gives sampling errors. Model uncertainty results from simplification of complex physical systems. Uncertainty can be reduced through improved measurements and improved model formulation.

Sensitivity analysis

Sensitivity analyses assess the effect of changes in individual model input parameters on model predictions. This is usually done by varying one parameter at a time and recording the associated changes in model response. One primary objective of a sensitivity analysis is to rank the input parameters on the basis of their influence on or contribution to the variability in the model output.

Uncertainty analysis

Uncertainty analysis involves the propagation of uncertainties and natural variability in a model's inputs to calculate the uncertainty and variability in the model outputs. It can also involve an analysis of the uncertainties resulting from model formulation. The contributions of the uncertainty and variability of each model input to the uncertainty and variability of the model predictions are explicitly quantified.

The EPA chose a staged approach for analysis of uncertainty and variability. The use of a staged approach has advantages for models as complex as TRIM.FaTE. The first stage, consisting of sensitivity analyses that are comparatively easy to implement, identifies influential parameters and generates an importance-ranking of parameters. The results of this stage are useful for narrowing down the number of parameters to be analyzed in the second-stage uncertainty and variability analysis and are also useful in evaluating model structure and modeling assumptions. The second stage involves uncertainty and variability analyses of increasing detail and complexity. Figure 6-1 illustrates this staged approach for the TRIM.FaTE module and how the functional parts fit together.

6.1 SENSITIVITY ANALYSES

The sensitivity analysis provides a quantitative characterization of the sensitivity of the model results to variations in the model input parameters. A ranking of sensitivity results can be used to provide a first-order determination of the most influential parameters that will need to be included in the detailed uncertainty analysis. Assessment of whether it is reasonable that parameters would have the influence they do in the model can also aid in evaluating model structure and modeling assumptions.

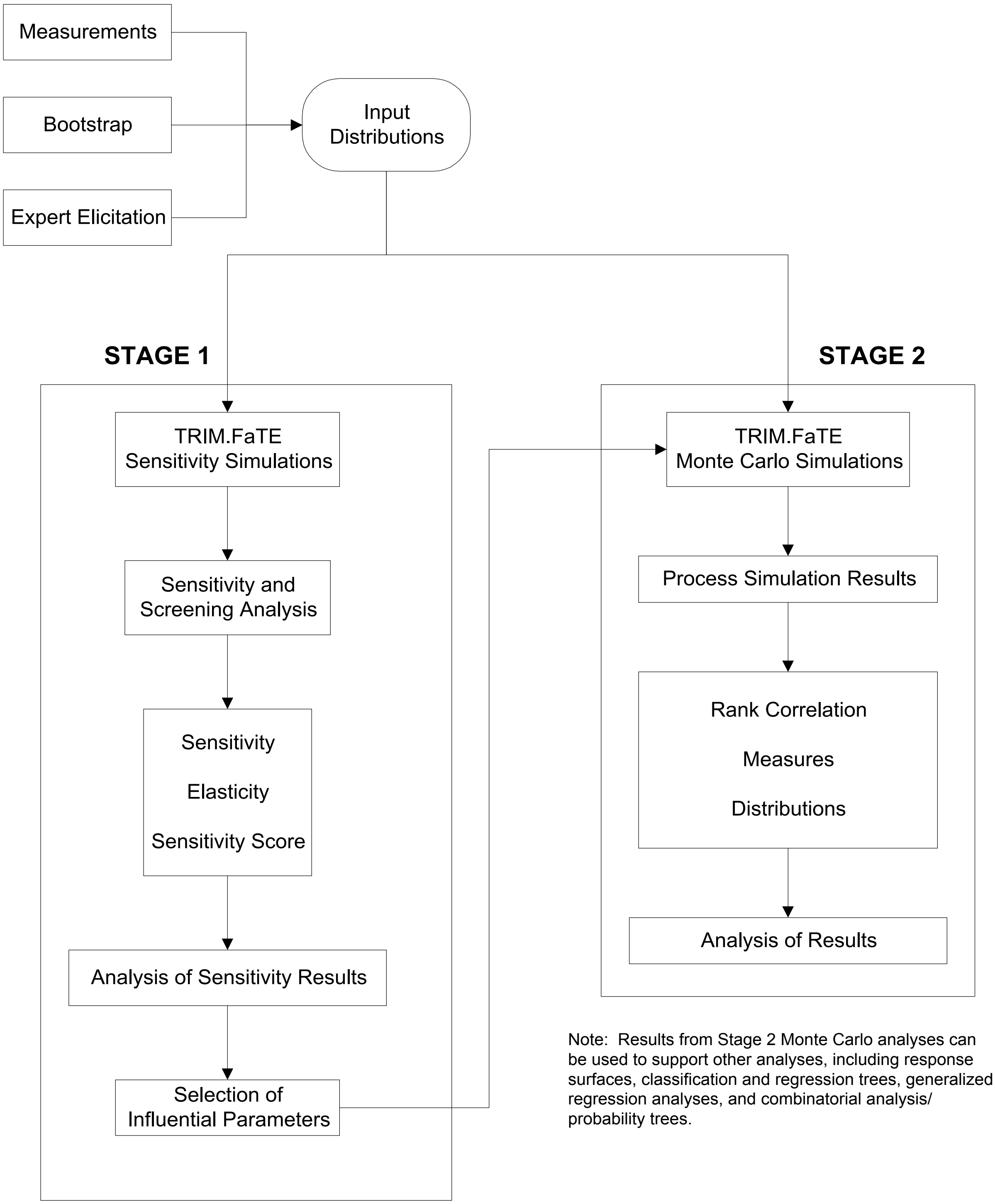
The TRIM.FaTE sensitivity feature allows the user to choose a set of parameters to vary, the compartments in which to vary them, and the compartments and chemicals for which the results are of interest. A parameter can be varied in parallel across all compartments of a specific type (*e.g.*, vary the organic carbon content in surface soil simultaneously for all surface soil compartments, where the varying parameter values would match across all surface soil compartments) or independently in specific compartments (*e.g.*, vary organic carbon content in surface soil separately for each compartment). One simulation of the user's design (*e.g.*, a 5-year dynamic run, or a steady-state analysis) is completed per selected parameter for comparison to the base simulation of the same design. All parameter values in that simulation would match the values in the base simulation except for the selected parameter which is set equal to a new value.

In the current version of TRIM.FaTE, the parameters to be varied must be constants or time-varying values such as meteorological data (*i.e.*, parameters that are specified by formulas in the model cannot be varied). The amount by which each selected parameter is varied (represented by) p) is specified by the user, and may be a small fixed percentage (*e.g.*, one to ten percent) of the nominal parameter value or a small fixed percentage of a measure of the spread of values the parameter typically addresses. One can use the standard deviation or a range of percentiles (*e.g.*, the range from the 10^{th} to the 90^{th} percentile). A simulation for each parameter is required for this analysis; thus, 2,000 simulations would be needed to examine 2,000 parameters.

For the selected compartment and chemical outputs of interest, the system will calculate the sensitivity score for each parameter based on a specified result (*e.g.*, the average concentration values for the last year of the simulations). Thus, the user may run simulations of the TRIM.FaTE model with the parameters being varied singly, with the model results summarized to show the sensitivity to parameters and to identify the most influential parameters.

The results of a sensitivity analysis are applicable to a particular location and for the range of conditions (*i.e.*, parameter space) simulated, and may not apply to conditions outside of this. To generate more broadly applicable sensitivity results, the sensitivity analysis can be performed for a number of different "nominal" base simulations representing distinct modeling regimes (*e.g.*, summer and winter time periods, wet and arid locations).

Figure 6-1
Uncertainty and Variability Analysis Framework
(Illustrated for TRIM.FaTE Module)



Varying parameters so that they are both larger and smaller by Δp (*i.e.*, varying by $\pm\Delta p$ instead of just $+\Delta p$) doubles the number of simulations required to complete the analysis, but allows the user to calculate the local nonlinearity of the effect of varying a parameter on the model results (*i.e.*, the nonlinear impact of varying parameters around a given value, for values close to the original value). These results are reported as second order terms in the sensitivity measures to show the extent of local nonlinearity for parameters. Non-local nonlinearities (*i.e.*, the nonlinear effects of wider variations of a parameter value) are quantified by increasing Δp to be in the range of 10 to 100 percent of the nominal values or spread of the parameters.

The results of these simulations are processed to produce measures of the importance of the parameters in the sense of how the model results change when the parameters are changed. The measures of parameter sensitivity and ranking automatically computed in sensitivity analyses are the *sensitivity,* the *elasticity*, and the *sensitivity score*. The user can set up sensitivity simulations to calculate the *nominal range sensitivity* if desired. We define these measures following Morgan and Henrion (1990).

The *sensitivity* of a model output to a parameter is the rate of change of the output with respect to changes in the parameter. Denoting the parameter as p and the model output as y, the sensitivity (at a particular value p^0 of p) is conventionally defined as the partial derivative $\partial y/\partial p$, evaluated at p^0. This measure describes how the model responds to small changes in the parameter p for values of p that are close to p^0, keeping all other parameters fixed, and is referred to as a "local" measure.

We calculate the sensitivity by:

$$Sensitivity = \frac{y(p^0+\Delta p) - y(p^0)}{\Delta p} = \frac{\Delta y}{\Delta p} \tag{14}$$

where Δp is a small change in the parameter value and:

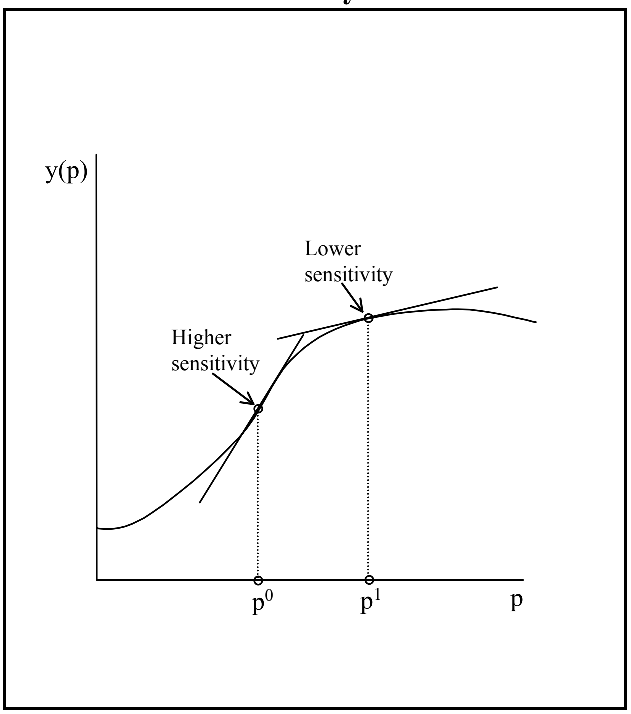
$$\Delta y = y(p^0+\Delta p) - y(p^0) \tag{15}$$

The *nominal range sensitivity* is used to assess changes in the model outputs resulting from large variations in input parameters. The effects on model outputs of varying each input parameter from the low end to the high end of the range of values for the parameter, are calculated in essentially the same way as the local sensitivity:

$$Nominal\ Range\ Sensitivity = \frac{y(p_{high}) - y(p_{low})}{p_{high} - p_{low}} \tag{16}$$

The sensitivity can be interpreted as the slope of the tangent to the response surface y(p) at the point p^0 (Figure 6-2). Note that the calculated value of the sensitivity depends both on the nominal parameter value p^0 and the amount of change) p. The sensitivity to a parameter can be quite different at different values p^0 of the parameter. It can be useful to vary both) p and p^0 to see how the sensitivity depends on them.

Figure 6-2
Illustration of Sensitivity in One Dimension



The *elasticity* is defined as the ratio of the relative change in the model output y to a specified relative change in a parameter p:

$$\textit{Elasticity} = \frac{\Delta y}{y^0} \Big/ \frac{\Delta p}{p^0} \tag{17}$$

where) p/p^0 is a fixed relative change. For example, if the specified parameter change is one percent ( ) $p/p^0 = 0.01$), then the elasticity is the percent change in y due to a one percent change in the parameter p, evaluated at a particular value p^0 of p.

The *sensitivity score* is the elasticity weighted by a normalized measure of the variability of the parameter which takes the form of a normalized range or normalized standard deviation of the parameter. The sensitivity score for the model input parameter p with respect to the model output y is defined as:

$$\textit{Sensitivity Score} \;=\; \frac{\Delta y}{\Delta p} \cdot \frac{\sigma}{\mu} \cdot \frac{p^{o}}{y^{o}} \tag{18}$$

where:

ªy/ªp	=	change in output y per change in input p
F/:	=	coefficient of variation of p (standard deviation/mean)
p^o/y^o	=	ratio of nominal values of the input and output

Other normalized measures of the variation of the parameter can be used in place of the coefficient of variation (*e.g.*, the range of p divided by the mean).

6.2 THE MONTE CARLO APPROACH FOR UNCERTAINTY AND VARIABILITY ANALYSES

A Monte Carlo approach with Latin Hypercube Sampling (LHS) is available within TRIM.FaTE for characterizing and analyzing the uncertainty and variability of the TRIM.FaTE outputs, with respect to the model inputs and parameters. The primary advantages of Monte Carlo methods for this type of analysis are the generality with which they can be applied, the lack of assumptions required, and their computational efficiency. Particular strengths of a Monte Carlo approach relevant to TRIM uncertainty and variability analyses include the following:

- Monte Carlo (MC) can be used to analyze many parameters.
- MC handles different ways of specifying parameter distributions.
- MC can treat correlations and dependencies.
- MC allows for tracking the propagation of uncertainty and variability through model components at any level.
- MC gives estimates of confidence bounds for the estimates of the output distributions.
- MC allows precision to be increased easily by performing additional iterations.
- LHS is an efficient sampling scheme, reducing the number of simulations required. (MC with LHS has computational complexity linear with the number of parameters or model inputs that are being analyzed.)
- MC handles complex algorithms in the model without increased difficulty.
- MC is flexible and will accommodate future additional analyses without major restructuring.

- MC output is compatible with a number of methods for specific analyses of uncertainty and variability, including response surfaces, regression models, classification and regression trees (CART), ranking methods, and combinatorial analysis.

- MC is widely used, is generally accepted in the scientific community, and can be explained to a lay audience.

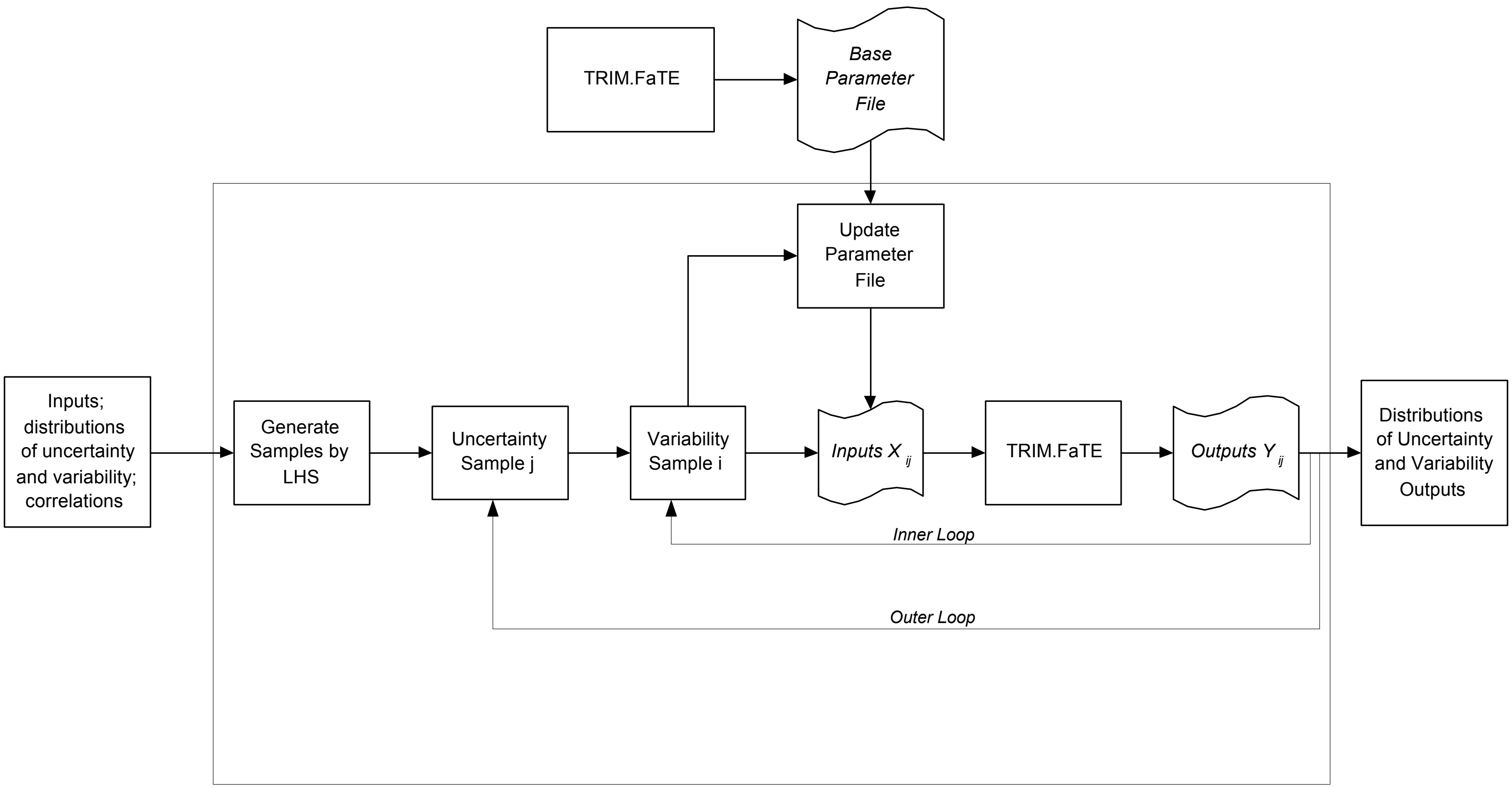
A significant limitation results from the fact that the analysis of uncertainty and variability requires estimates of parameter distributions that reflect both uncertainty and variability individually, and information on the distributions for parameters is not available for most parameters. Estimates of dependencies (*i.e.*, correlations) between parameters would enable a more detailed analysis to be performed, although this is of lesser importance. However, when a parameter distribution has been developed, it is rarely separated into components of uncertainty and variability. This limitation of the Monte Carlo approach can be addressed by developing distributions for the parameters to which the model shows the greatest sensitivity. Distributions are not needed for all parameters.

6.2.1 TWO-STAGE MONTE CARLO DESIGN

Two-stage Monte Carlo designs are used to characterize uncertainty and variability separately. This is not currently implemented in TRIM.FaTE, and is being considered for a future version. Joint uncertainty and variability Monte Carlo simulations are generated based on sampling from an uncertainty distribution and a variability distribution for each parameter, with the uncertainty distributions sampled in an outer loop and the variability distributions sampled in an inner loop. For each uncertainty realization (outer loop sample) there is a specified distribution of variability (for each parameter) from which several samples are drawn to represent variability in the inner loop. These several samples represent one variability realization. Figure 6-3 illustrates the structure of this two-stage Monte Carlo design.

As an example, suppose there are N_u samples drawn from the uncertainty distributions, and that for each uncertainty sample there are N_v variability samples. The cumulative distribution function (of a model output) representing variability for that uncertainty sample can be estimated from these N_v variability samples and statistics can be calculated (*e.g.*, mean, percentiles, variance). For each of these statistics, there are N_u values, corresponding to the N_u uncertainty samples. These are then used to calculate a cumulative distribution function for each statistic, representing the uncertainty distribution for that statistic.

Figure 6-3
Two-stage Monte Carlo Approach



6.2.2 DISTRIBUTIONS OF INPUT PARAMETERS

The Monte Carlo approach requires specification of probability distributions for each parameter being analyzed for its role in the overall uncertainty of the model. In general, distributions can be specified as parametric forms of probability distribution functions (PDFs) or cumulative distribution functions (CDFs), as nonparametric PDFs or CDFs, or as sets of data points from which samples are drawn. At the present time the distributions supported by TRIM.FaTE are the uniform, normal, lognormal and triangular distributions. Future enhancements to TRIM.FaTE will include an expansion of the types of distributions which can be specified by the user.

Distributions for parameter variability and for parameter uncertainty are required for those parameters to be analyzed; TRIM does not use "default" distributions where there is no information. Parameters without any specification of distributions are treated as if they are known exactly.

6.2.3 LATIN HYPERCUBE SAMPLING

There are four sampling techniques that are widely used in Monte Carlo methods for generating random samples from parameter distributions: simple random sampling, Latin hypercube sampling (LHS), midpoint LHS, and importance sampling. Randomness is an important feature of these methods for sampling, since it allows one to directly estimate the precision of the statistics estimated using the Monte Carlo approach.

Both the simple random sampling and LHS techniques are available in TRIM.FaTE. The preferred sampling technique is LHS, which employs a stratified random sampling without replacement scheme that is very efficient for sampling, especially for multiparameter models (Iman and Shortencarier 1984, Iman and Helton 1987, Helton and Davis 2000). Importance sampling strategies also will be used in conjunction with LHS to obtain better coverage of distribution tails or extreme values. The strata for LHS are chosen to be intervals partitioning the range of each parameter, in such a way that the parameter has equal probability of realization within each interval. Then a sample is selected randomly from each of the intervals. To illustrate this, say there are k intervals used for each parameter. A random sample is selected from within each interval, and this is repeated for each parameter, yielding k samples for each parameter. Then, k multivariate samples are constructed by randomly pairing up the samples for each parameter. These k sets of parameter values (each set containing a value for each parameter) are referred to as the Latin hypercube sample.

If there are correlations among the parameters, there is a technique for sampling within the LHS framework so that the sample reflects the correlations (Iman and Conover 1982, Iman et al. 1985). This treatment of correlation is based on rank-order correlation (Kendall and Gibbons 1990) and has desirable properties. It can be used with any distribution and with any sampling scheme, and it does not change the marginal distributions of the parameters. This is being considered for inclusion in a future version of TRIM.FaTE.

6.2.4 TREATMENT OF TAILS OF DISTRIBUTIONS

As noted above, for certain influential parameters an importance sampling technique will be incorporated to obtain adequate sampling coverage of extreme values of these parameters. Importance sampling refers to a class of sampling techniques that takes into account the areas of a distribution that are important to the analysis, providing enhanced detail in these areas. Importance sampling is often used when increased accuracy in one or both tails of a distribution is desired. These techniques are being considered for a future version of TRIM.FaTE.

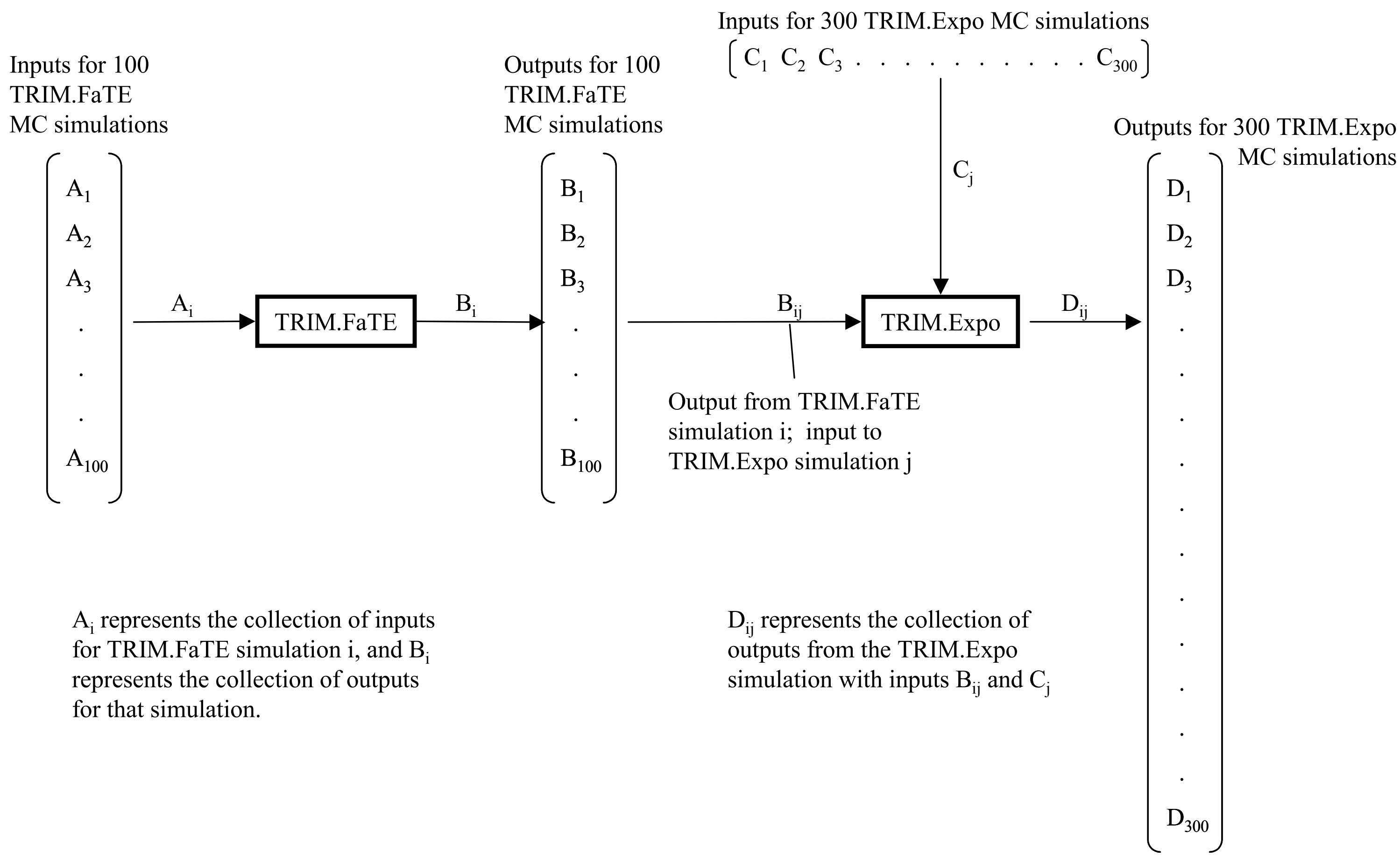
6.2.5 TRACKING INFORMATION BETWEEN MODULES

There are two levels at which tracking of information related to uncertainty analysis occurs; the first is within each TRIM module, and the second is from one TRIM module to the next. The information passed from one TRIM module to the next (*e.g.*, from TRIM.FaTE to TRIM.Expo) needs to provide enough detail to allow for continuation of the Monte Carlo propagation of uncertainty and variability in the next module. Information on the joint distributions of a TRIM module's inputs and outputs is required to do this, for both uncertainty and variability. This is accomplished by maintaining a record of the input parameter values used for each Monte Carlo simulation of a TRIM module. Simulations of one module are randomly selected for input to Monte Carlo simulations for a succeeding module, while keeping track of the input values for all simulations.

For example, take the first module to be TRIM.FaTE and the following module to be TRIM.Expo. TRIM.Expo takes as inputs some of the results generated by TRIM.FaTE, in addition to other input parameters. Suppose that 100 Monte Carlo simulations of TRIM.FaTE are performed and, following this, TRIM.Expo is going to be run for 300 Monte Carlo simulations. Figure 6-4 provides an illustration of this example. For each of the TRIM.Expo Monte Carlo simulations, one of the TRIM.FaTE simulations is randomly selected and the results of this simulation used for input to TRIM.Expo. There are other input parameters also input to TRIM.Expo, and some of these might be sampled from uncertainty and/or variability distributions as part of the Monte Carlo process. Using the notation of Figure 6-4, suppose the i^{th} TRIM.FaTE simulation is selected for the j^{th} Monte Carlo simulation of TRIM.Expo. For this simulation, TRIM.FaTE inputs $\{A_i\}$ result in outputs $\{B_i\}$ which are then input to TRIM.Expo. The other inputs to the j^{th} Monte Carlo simulation of TRIM.Expo are denoted as $\{C_j\}$, and the results of this simulation are denoted as $\{D_j\}$. Then, each of the 300 simulations of TRIM.Expo are tagged with the indices i_j and j to respectively track the corresponding TRIM.FaTE and TRIM.Expo input values, for j = 1 to 300. The index *I* takes values from 1 to 100, but is indexed by *j* so that the TRIM.FaTE inputs used for the j^{th} TRIM.Expo simulation are tracked.

The same process would be used for a module following TRIM.Expo, where the 300 TRIM.Expo simulations would be tagged by i_j, j = 1 to 300.

Figure 6-4
Example of Propagation of Uncertainty and Variability Between TRIM Modules



Care must be taken to ensure that the model input values are consistent in sequences of runs. For example, if there is an input to TRIM.FaTE which is also an input to TRIM.Expo, then the value for the TRIM.Expo simulation should be the same as the TRIM.FaTE input value. Similar consistency constraints should be imposed if joint variables are highly correlated or related by a functional relationship.

6.2.6 COMPUTATIONAL RESOURCES

Although the Monte Carlo technique is very efficient, Monte Carlo simulations of TRIM.FaTE require substantial computer processing time, especially when treating more than a few parameters. The available computational resources can be a limiting factor in the scope of the analysis performed. Consequently, the more detailed analyses may have to restrict their scope to small numbers of parameters being jointly varied.

Computer processing time for both the uncertainty propagation and tracking and the TRIM.FaTE model depends on the definition of the TRIM.FaTE modeling scenario, in terms of the numbers of compartments, time steps, length of simulation, chemicals, and so forth. It also depends on the number of parameters and number of model outputs analyzed, the sizes of the Monte Carlo samples (which relates to the number of simulations), and the level of detail of the analysis.

Uncertainty analyses may be conducted running TRIM.FaTE in a steady-state mode, which requires drastically less processing time than the dynamic modeling mode. In the steady-state mode, TRIM.FaTE calculates single values for chemical moles, mass, and concentration for each compartment. These values approximate the steady-state levels that the chemical would reach if the dynamic form of the model was run for a long enough period of time to allow all chemical mass inputs and outputs to balance for each compartment (*i.e.*, to reach a steady-state).

6.2.7 SPATIAL AND TEMPORAL RESOLUTION AND AGGREGATION

Estimation of the effects of spatial and temporal aggregation on uncertainty and variability could be accomplished by sensitivity analyses of Monte Carlo results. For analysis of spatial aggregation, the user could set up a small number of TRIM.FaTE scenarios with increasing levels of spatial resolution (decreasing levels of aggregation), and run the same set of simple Monte Carlo simulations for each scenario. Comparison of the Monte Carlo output distributions for the scenarios would show the impact of the aggregation on uncertainty and variability for the scenarios modeled. Similarly, the effects on model output uncertainty of temporal aggregation could be assessed by comparing uncertainty results from scenarios with different levels of temporal aggregation.

6.2.8 SPECIFICATION OF PROBABILITY DISTRIBUTIONS OF MODEL INPUTS

The need for distributions for the input parameters is discussed above. Implementation of this Monte Carlo approach employs a data file that specifies the distributions of uncertainty and variability for each parameter. For each parameter, this file contains the distribution name *(e.g.*, lognormal) and the parameters or data that complete the specification of the distribution. A distribution for variability and a distribution for uncertainty is required for each parameter. As described in Section 6.2.1, both variability and uncertainty distributions are used a two-stage Monte Carlo analysis.

There are often physical constraints on values of parameters and intermediate quantities in the model; for example, mass is always non-negative. These can have implications for how parameter distributions are set. The specified distributional forms should satisfy the physical constraints as well as reflect the distributions indicated by the available data.

6.3 PRESENTATION OF UNCERTAINTY RESULTS

When a model has many inputs and is complex, as TRIM.FaTE is, the analyst will make use of methods that are simple and give a first-order picture of uncertainty, as well as more complex methods giving a more refined, detailed analysis of uncertainty. There are several ways to form summary measures and present the uncertainty and variability of a modeling system. Loosely speaking, "measures" are one or a small number of descriptive statistics, such as the sensitivity score, or the 10^{th}, 50^{th}, and 90^{th} percentiles of a distribution. In addition to summary measures, ways of presenting the results include graphs of distributions of model outputs, tree diagrams, other graphs, and tables of statistics.

Results from Monte Carlo simulations are collected in a data file which can be accessed with other analysis software, such as graphical and statistical software, to analyze and present the results of the uncertainty and variability analysis. In the future, the overall TRIM framework or TRIM.Risk may be used to generate these results:

- Sensitivity
- Sensitivity score
- Elasticity
- Probability density functions
- Cumulative distribution functions
- Confidence intervals
- Tables of statistics
- Rank order correlation
- Correlation matrix
- Scatter plots, scatter plot matrix

The first three of these are produced from results of the sensitivity simulations; the remainder can be produced from the Monte Carlo results.

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