3. TREATMENT OF UNCERTAINTY AND VARIABILITY IN TRIM

This chapter summarizes the approach for assessing uncertainty and variability in the TRIM modules. Additional background on how this method was selected is provided in Appendix B of this report. A specific discussion of the approach for TRIM.FaTE is presented in Chapter 6 of TSD Volume I. The following text box presents definitions for the key terms used in this chapter to explain the uncertainty and variability analysis framework for TRIM.

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 (taking more precise measurements of people's heights does not reduce the natural variation in heights). However, it can often be reduced by a more detailed model formulation (*e.g.*, modeling people's heights in terms of age will reduce the unexplained variability of heights).

Uncertainty

Uncertainty refers to the lack of knowledge regarding the actual values of physical 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

Sensitivity refers to the rate of change of the model output with respect to changes in an input parameter.

3.1 OBJECTIVES OF THE INTEGRATED UNCERTAINTY ANALYSIS

Development of the TRIM framework involved development of an approach to estimate uncertainty and variability in a manner that allows for integration between the TRIM modules and for tracking the uncertainty and variability through the modules. The TRIM approach for uncertainty and variability analysis is intended to accomplish the following objectives:

- Propagation of variability, uncertainty, and parameter dependencies throughout TRIM in an integrated manner, tracking uncertainty and variability jointly and separately;
- Characterization of uncertainty and variability of model results with respect to parameter distributions and correlations, and calculate summary measures of the uncertainty and variability of model results that clearly convey the important aspects of model uncertainty and variability;

- Identification of critical parameters and correlations through sensitivity analyses;
- Information to guide data improvement efforts (including setting priorities for gathering data to develop distributions of parameters), guide model simplification efforts, and support temporal and spatial aggregation choices;
- Results that can support risk management decision-making; and
- Estimation of uncertainty and variability within a reasonable amount of computer processing time.

3.2 GENERAL STEPS IN AN ANALYSIS OF UNCERTAINTY AND VARIABILITY

The analysis of uncertainty and variability in a risk assessment takes place through a series of functional steps. Some steps may be skipped and others may be incorporated in more sophisticated or refined iterations. Underlying the risk assessment is a mechanistic model of the risk process. In the case of the TRIM.FaTE module of TRIM, the model algorithms represent the physical and chemical processes that transfer chemical mass through different compartments of a physical system. As a first step, the mechanistic model can be evaluated in a deterministic manner for its sensitivity to changes in its variable inputs. For example, one very simple sensitivity analysis looks at the percent change in the model output (*e.g.*, risk) given percent changes in model inputs (*e.g.*, emissions, wind velocities, air-to-soil deposition rates, soil density). This technique does not require information about the range of values of the input variables, but requires only a selection of possible single values from which local deviations are calculated. This univariate analysis can be expanded to look at pairs of input variables, thereby taking into account dependencies or interactions between variables. Such simple analyses of model sensitivity are valuable because they can be used quickly and easily to identify the variables that have the greatest potential to "influence" the model results, based on the relationships in the model and the selected set of values.

The second step of the analysis is collecting information about the ranges and likelihoods of the values the variables might take. After the ranges are estimated for the variables, it is possible to conduct a deterministic scenario analysis by selecting a set of values for each variable and using the mechanistic model to calculate risk for each possible combination of the selected values. A probability tree can be created by adding information about the likelihood of each scenario. Either approach can be implemented to identify the most important variables on the basis of the combination of model response sensitivity and indeterminancy (*i.e.*, lack of knowledge of the actual or "true" values) in the variables. A variety of approaches are available to estimate the ranges and likelihoods of the values for the input variables. Examples include direct measurement of the physical system and elicitation of expert judgment. Further processing of the input data may be desirable to fit analytical forms, such as normal or lognormal probability distributions, or to estimate statistics, such as the mean and variance, from the information about the dispersion in the variable values. The bootstrap is a statistical resampling method that can assist with this step (Efron 1980).

The propagation of uncertainty and variability in a very simple mechanistic model may be conducted through combinatorial methods, including the sensitivity analyses described above, discrete probability trees, and analytical approaches such as the method of moments, Taylor series expansions, and differential analysis. An alternative to these approaches is Monte Carlo simulation, using either simple or stratified random samples from the input probability distributions to approximate the output distribution for risk. The Monte Carlo approach was selected for TRIM uncertainty and variability analysis. The selection of the Monte Carlo approach does not exclude the use of the other approaches. In fact, Monte Carlo was selected because it provides flexibility. If input values can be tracked along with the results of each iteration, these data can be used in the other approaches.

If the mechanistic model is very complex, computational resources may be conserved by "modeling the model." One option for this approach is to develop a response surface by simulating a very large number of scenarios, as in the combinatorial approach described above, and fitting a surface to the results using regression techniques. This response surface model can be substituted for the mechanistic model when propagating uncertainty and variability. Alternative methods for "modeling the model" include generalized linear models and other regression models; the class of fuzzy logic, neural networks, and genetic algorithms; and a technique known as classification and regression trees (CART). Any of these approaches can be used to reduce the form of the mechanistic model to dramatically reduce the time required to compute the risk results for large numbers of scenarios or samples in a Monte Carlo application. These approximations to the model are called "reduced form models." Drawbacks to using reduced form models include inaccuracies (because they are only approximations) and the restriction of not extrapolating outside of the scope of the simulations performed to build the reduced form model.

A final step in the analysis of uncertainty and variability is the interpretation of the relationship between the distributions of the results of the model and the distributions of the model inputs. Distributions of model results can be prepared and presented as part of the risk characterization module, TRIM.Risk (see Chapter 9), either directly or interpreted in terms of identifying important assumptions and parameters, which are also presented in TRIM.Risk. Much like the deterministic tests of the sensitivity of the model to local changes in the inputs, tests can be constructed to identify the probabilistic importance of the indeterminate variables. The first step in accomplishing this is to calculate a sensitivity score composed of the elasticity, the coefficient of variation, and the ratio of nominal input and output values. This score considers the range of uncertainty in the variables and the change in output per change in input, and it also identifies variables with both relatively high sensitivity in the model and high dispersion. Additional approaches for calculating and presenting measures of uncertainty include rank correlation, analysis of deviance, confidence intervals, distributions of the model outputs, and joint distributions of the model parameters and outputs.

3.3 OVERVIEW OF THE APPROACH SELECTED FOR TRIM

There are numerous expositions in the published literature describing techniques and applications of analysis of uncertainty and variability. Several techniques are used in a wide range of disciplines, including ecological risk assessment, manufacturing, aerospace applications, and nuclear physics. Respected references related to risk analysis include Beck (1987), Cohrssen and Covello (1989), Cullen and Frey (1999), Morgan and Henrion (1990), National Research Council (1994, 1996), and Vose (1996).

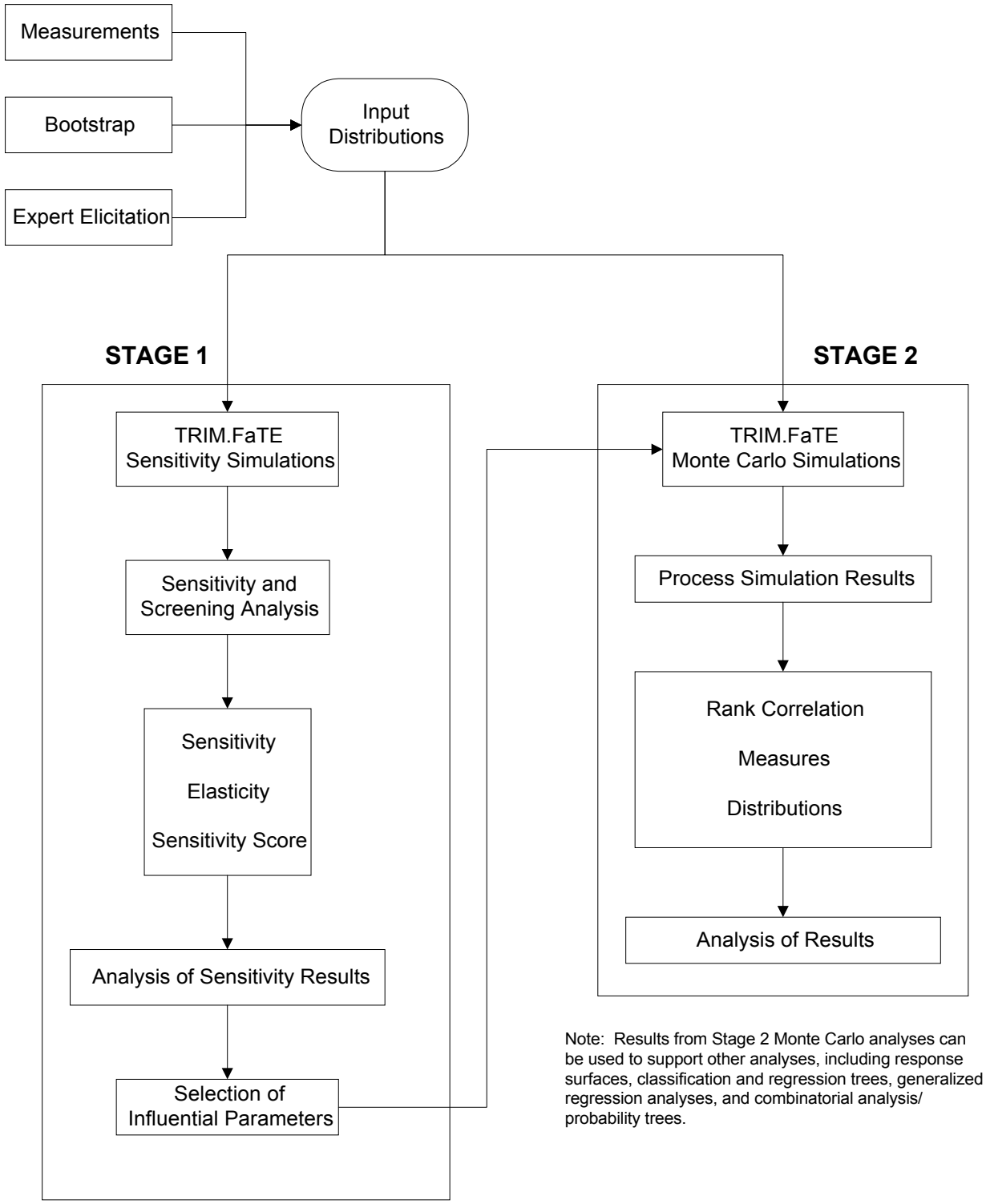
In agreement with EPA guidance on probabilistic assessments, OAQPS chose a staged approach for analysis of uncertainty and variability in TRIM. The use of a staged approach has advantages for models as complex as TRIM. The first stage consists of analyses that are comparatively easy to implement, identifying influential parameters and giving an importance-ranking of parameters, which are useful for narrowing down the number of parameters to be analyzed in the uncertainty and variability analysis. This first stage is considered a sensitivity and screening analysis. The second stage involves uncertainty and variability analyses of increasing detail and complexity. Figure 3-1 illustrates this staged approach and how the functional parts fit together. This approach provides the TRIM user with options to perform a sensitivity analysis or a combined sensitivity and uncertainty/variability analysis, where the sensitivity results guide the selection of parameters for the uncertainty and variability analysis. The user also has the option to perform only the uncertainty and variability analysis, if the user has identified specific parameters to analyze.

The sensitivity and screening analysis calculates the importance of parameters with respect to how the model results change when the parameters vary, varying parameters singly or in pairs. This process provides for a first-order determination of the more influential parameters and allows further analysis to focus on the key parameters.

The screening component of this approach is performed to narrow down the scope of the second-stage detailed analysis, in terms of the number of parameters to be treated, by identifying influential parameters which should be retained for further analyses. This is a critical step toward the goal of producing a economical representation of uncertainty and variability, excluding less influential terms and parameters and still capturing all of the significant features of TRIM uncertainty and variability.

A Monte Carlo approach was selected for the second stage, the detailed uncertainty and variability analyses. Monte Carlo methods for analysis of model uncertainty use statistical sampling techniques to derive statistics that characterize uncertainty. Essentially, a Monte Carlo approach entails performing many model runs with model inputs randomly sampled from specified distributions for the model inputs. Using a two-dimensional Monte Carlo simulation, uncertainty and variability can be modeled separately. These model runs can be set up to characterize the propagation of uncertainty and variability of the model input parameters, taking into account distributions of parameter uncertainty and variability and parameter dependencies. These simulations provide uncertainties of model outputs in terms of distributions of model

Figure 3-1
Uncertainty and Variability Analysis Framework
(Illustrated for TRIM.FaTE Module)



outputs, joint distributions of model inputs and outputs, and summary scalar measures. These are the core data from which information about uncertainty and variability can be extracted.

While the importance of characterizing uncertainty and variability explicitly and separately is well recognized (NRC 1994, CRARM 1997, U.S. EPA 1997c), this does not imply that OAQPS will do so for all cases and all parameters. As stated above and described below, TRIM will have the capability of evaluating and tracking uncertainty and variability separately via two-dimensional Monte Carlo simulation. However, the parameters for which this will be done will be determined on a case-specific basis. The OAQPS intends to characterize uncertainty and variability separately only for critical parameters and where appropriate based on the underlying science and data.

The analysis of uncertainty and variability requires estimates of the distributions of parameters, reflecting both the uncertainty and variability of the parameters in question. In addition, estimates of dependencies (correlations) between parameters would enable a more detailed analysis to be performed. However, typically data are not collected or measured in a way that allows for separating uncertainty and variability for most parameters. When a parameter distribution is available, it is rarely separated into components of uncertainty and variability. For some parameters, such as body weight, the inherent variability within a population has been characterized through the use of large surveys and precise measurement methods. However, emission rates, such as stack gas sampling, have been measured in such a way that separating uncertainty and variability is not supported by the data and would require more of a numeric exercise to tease out variability based on assumptions which may themselves introduce unspecified uncertainty. In some cases, this exercise may result in introducing uncertainty to a greater degree than the variability that is estimated.

This is a current limitation of the Monte Carlo approach which can be addressed over time by developing distributions for parameters to which the model is most sensitive. It should also be noted that OAQPS intends to conduct probabilistic analysis in a tiered approach in accordance with EPA guidance (U.S. EPA 1997b). First, critical parameters are identified through sensitivity analysis, distributions are developed, and correlations are identified only for the more critical parameters. Therefore, distributions are not needed for all parameters for either composite uncertainty or uncertainty and variability separately.

The analysis of the TRIM predictions of risk involves the propagation of uncertainty through the TRIM modules. This can be accomplished by conducting a two-stage analysis of uncertainty and variability sequentially for each of the TRIM modules. The distributions of outputs are passed from one module to the next to propagate distributional information to succeeding modules.

Because the amount of data produced from Monte Carlo simulations is voluminous, the full results will be archived and a reduced set will be retained to feed the next module. The output values from each of the TRIM modules as well as the model inputs (parameter values) for each Monte Carlo simulation will be saved. This large amount of information could be passed along to the next module for subsequent uncertainty analysis, but the amount of data would increase drastically from one module to the next. As illustrated by Figure 3-2, the output data

($B_1|A_1, A_2...A_n|$) from Module I (*i.e.*, TRIM.FaTE) also are part of the input data to Module II (*i.e.*, TRIM.Expo), and a portion of the input data to Module II (B_1) is dependent on the input parameters to Module I (A_i). The notation $B_1|A_1, A_2...A_n|$ indicates the dependence of the module outputs B_1 on the module inputs A_1, A_2, ...A_n. Module II also has input data from different sources, as represented by B_2 through B_n. Similarly, the output data from Module II ($C_1|B_i|A_i||$) are dependent, in part, on the input parameters to both Module I and Module II. Therefore, it is important to track the input parameters to each TRIM module. However, Figure 3-2 only depicts the information flow for a single simulation, and the actual volume of information would be multiplied by the number of Monte Carlo simulations performed (potentially thousands).

To reduce the size and complexity of the flow of uncertainty and variability information between TRIM modules, these results will be summarized in the form of nonparametric probability distributions that can be passed to the next module, where each distribution to be passed is characterized nonparametrically by its percentiles. Figure 3-3 illustrates how input parameters and output data will be tracked as distributions.

Another way in which the amount of information to be tracked through the modules can be reduced is through the use of the screening and sensitivity stage analysis described above. The simulation could be run with this feature to select the critical parameters in each module to be tracked for the more detailed uncertainty analysis; all other parameters would be set at their central tendency value in the more detailed analysis run. To further reduce the volume of information, after summarizing the results from one module as probability distributions, the transmission of information to the next module is filtered to select the most critical parameters (*e.g.*, those that account for 95 percent of the variance of the uncertainty and variability).

The Agency has begun testing the two-stage approach to uncertainty and variability described in this section as part of the TRIM.FaTE mercury case study (described in Chapter 7). These tests involve the uncertainty analysis for one module and not for a sequence of modules, as depicted by the outlined area in Figure 3-3. When the TRIM modules are linked together, each module after the first will treat its inputs from the previous module in the same way its other inputs are treated, as deterministic values with uncertainty and variability distributions. Therefore, no modification to the approach that OAQPS is testing for TRIM.FaTE is required for the remaining modules, and the extension to other modules will be straightforward.

Figure 3-2
Information Flow for a Single Monte Carlo Simulation of TRIM

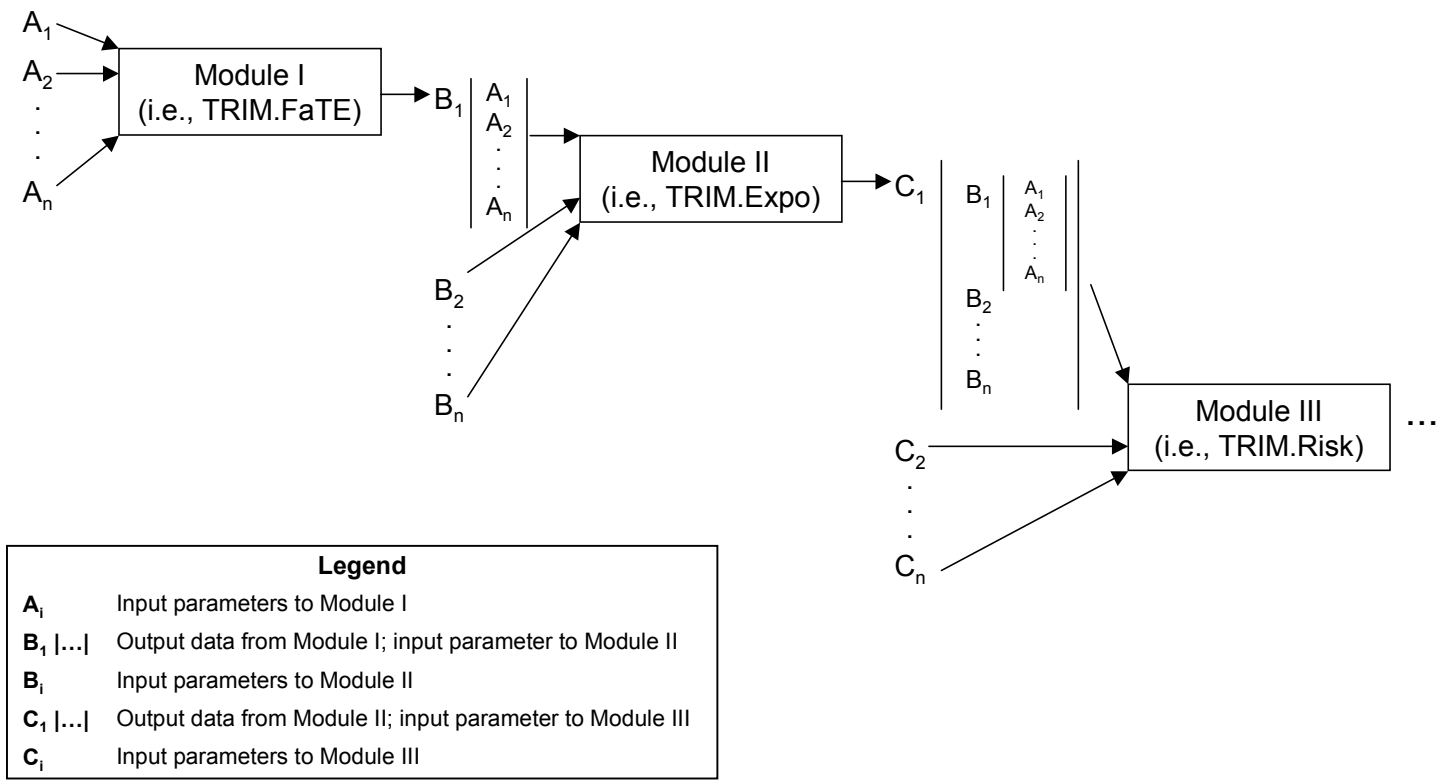
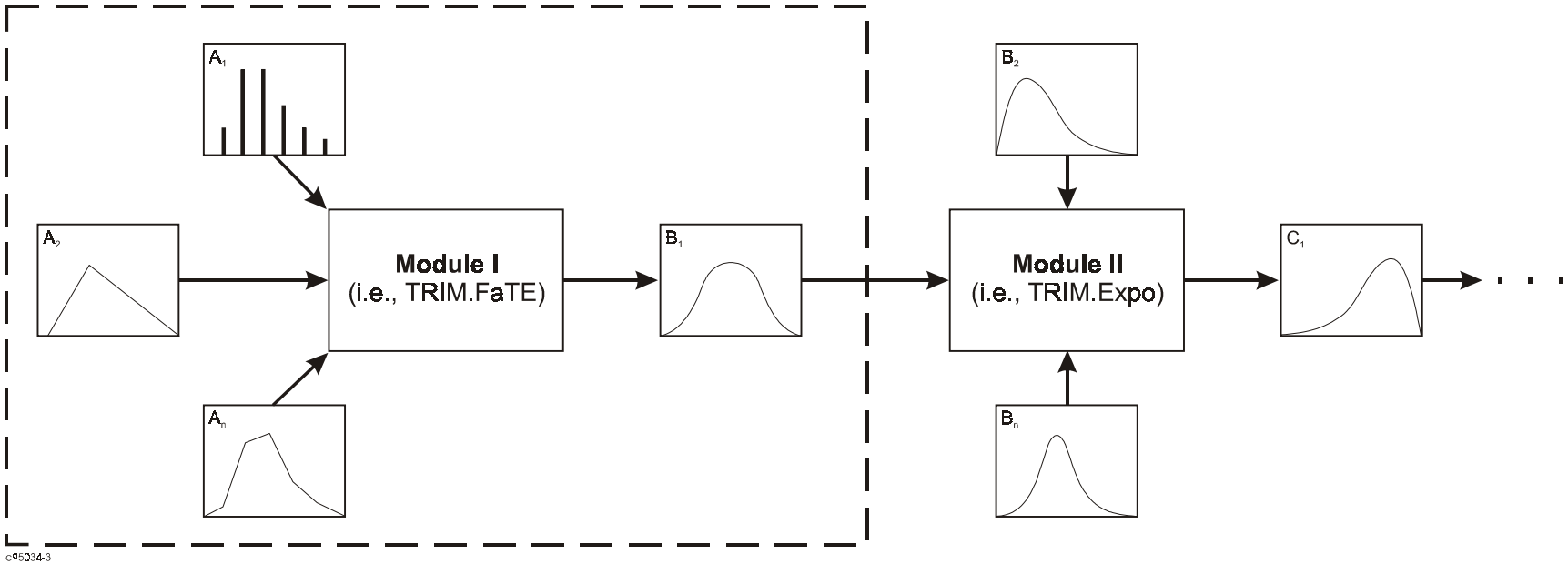


Figure 3-3
Nonparametric Probability Distribution Method for Information Flow in Monte Carlo Simulation



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