Using Monte Carlo Analysis in Ecological Risk Assessments

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Abstract

Monte Carlo analysis is a statistical technique for risk assessors to evaluate the uncertainty and variability associated with risk assessments for contaminated sites. The objective of this paper is to review how Monte Carlo analyses might be used in ERAs and to provide guidelines for determining the applicability of Monte Carlo analysis to certain situations. Terms that are pertinent to Monte Carlo analysis are provided, together with explanations of what Monte Carlo analysis is and the types of information needed to conduct such an analysis. Important considerations that need to be weighed before incorporating a Monte Carlo analysis into an ERA are presented and regulatory requirements are summarized.

Introduction

Monte Carlo analysis is a method that uses statistical sampling techniques to derive the probabilities of possible solutions for mathematical equations or models. One use of Monte Carlo is to evaluate the probability of particular outcomes from risk assessment modeling. Monte Carlo analysis could become increasingly important as a means for risk assessors to evaluate the uncertainty and natural variability associated with risk assessments for contaminated sites. For this reason, regulatory agencies have developed guidance for incorporating Monte Carlo analyses into human health and ecological risk assessments (ERAs) and that guidance is continuing to evolve. Many project managers have encountered the term Monte Carlo analysis at some point and wondered whether it is something that could be useful for their risk assessments.

This report addresses the use of Monte Carlo methods for conducting probabilistic ERAs. Although much of the material may also be pertinent to the use of Monte Carlo analyses in human health risk assessments, the focus will be on the use of Monte Carlo analyses in ERAs. Specifically, this document provides information about what Monte

Carlo analysis is, how Monte Carlo analysis is performed, when Monte Carlo analysis may or may not be appropriate for use in an ERA, and the regulatory requirements pertaining to the use of Monte Carlo analysis in ERAs.

What is Monte Carlo Analysis?

Monte Carlo analysis is a method initially developed in the 1940s that uses statistical sampling techniques to obtain a probabilistic approximation to the solution of a mathematical equation or model. As such, it is a tool that can be used for conducting probabilistic risk assessments. A probabilistic risk assessment is an assessment that estimates the probability or likelihood that particular risk values would result from exposure to contaminants at a site. In the context of an ERA, a probabilistic risk analysis involves the use of methods for estimating the probability that ecological receptors will be harmed by environmental contaminants. Although there are some ERAs where probabilistic analyses have been included, all ERAs are required to calculate a single value or "point estimate" for evaluating whether a contaminant will harm a particular ecological receptor (e.g., a hazard quotient). When single values are used to describe risks in an ERA, it is known as a deterministic risk analysis. In a deterministic risk analysis, it is implied that the determined risk values adequately represent the risks to organisms and little or no information is provided about the *probability* that a particular value will result from exposure to a site's contamination. Monte Carlo analysis is used to determine the probability of occurrence for the entire range of point estimates of a deterministic risk assessment and, in this way, deal with the uncertainty associated with these assessments.

To facilitate the discussion about how a Monte Carlo analysis is performed, some basic terms are defined in the following sections.

Uncertainty and Variability

One of the primary reasons to use a Monte Carlo analysis would be to examine the effect of uncertainty and natural variability on the estimate of risk. Uncertainty refers to a lack of knowledge about specific factors, parameters, or pathways. For example, a risk assessor may be uncertain about the concentration of a specific contaminant or the rate of contaminant uptake by the ecological receptors at the site. Uncertainty could be the result of measurement error, sampling error, model uncertainty (uncertainty due to simplification of real-world processes, incorrect model structure, misuse of models, and use of inappropriate assumptions), descriptive errors, aggregation errors, and errors in professional judgement. Since uncertainty refers to things that are unknown or unsure, the collection of additional site-specific information can reduce the degree of uncertainty.

Variability, on the other hand, refers to the differences in measurements or responses that are due to the true heterogeneity or diversity in a population or exposure parameter. Variability, usually measured as standard deviation or variance, represents natural random processes that can stem from environmental, lifestyle, and genetic differences among individual organisms. Examples of natural variation include physiological variation (e.g., variation in body weight, inhalation rates, drinking rates, and feeding rates), and variation in soil moisture across a site. Variation in contaminant concentrations at a site can also contribute to the variability in responses from ecological receptors exposed to a particular site. Variability cannot be reduced through additional measurements or studies, although the uncertainty of variability (i.e., how precisely the variability is known) can be improved.

For example if we were to examine the body weight for a portion of the individuals of a particular species (e.g., white-footed mice) at a site, we would find a range of body weights. The distribution of body weights in the mouse population could be described statistically using the mean, the range, and the standard deviation of the sampled weights. Additional sampling would not change the natural variability in the body weights, although the uncertainty for our statistical description (e.g., the mean) of the body weights would decrease as we increased the sample size. Theoretically, if we perfectly weighed all of the mice at the site, there would be no uncertainty in the mean value (or any other descriptive statistic, for that matter) assigned to body weight, yet variability in the population would remain.

Probability Density Functions

Because of uncertainty and variability, the value for many environmental variables cannot be known until a direct observation is made. Consider, for example, the weight of a mouse taken at random from the mouse population described in the previous section. There is no way to know the exact weight of that mouse until it is weighed. Similarly, the exact concentration of a contaminant in a sample from a site is not known until the sample has been analyzed. However, if samples of these parameters had been previously made, statistical information could be used to help us make a guess about the likely value for a randomly collected sample. The variability for a parameter can be represented as a probability density function (PDF), alternatively referred to in the literature as a probability function, frequency function, or frequency distribution. An example of a PDF is shown in Figure 1. For a continuous variable (a variable that can assume any value within some defined range) the probability density function expresses the likelihood that the value for a random sample will fall within a particular very small interval. For discrete variables, that is variables that can only assume certain isolated or fixed values (e.g., a roll of a dice or the toss of a coin), the term probability mass function is sometimes preferred over the term PDF. The PMF expresses the probability that a randomly selected discrete variable will be a specific value.

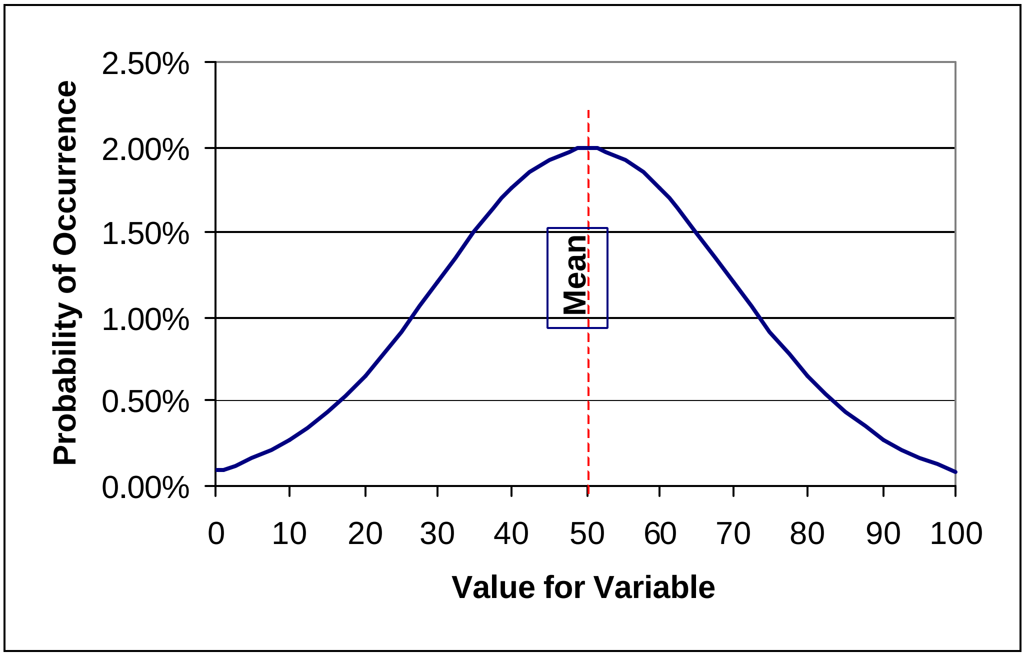

Figure 1. Example of a probability density function.

Probability density functions are used as the basis of a Monte Carlo analysis and the proper selection of PDFs to represent the variability of the input parameters is essential to a meaningful analysis. Probability density functions can take on a variety of shapes. Examples of some theoretical PDFs include normal, lognormal, exponential, uniform, Poisson, and binomial distributions and each of these has distinctive characteristics (Figure 2). In addition, custom probability functions that do not fit any of the theoretical distributions can be derived for a particular parameter by using the frequencies at which particular values for the parameter are observed. The PDF selected for each input parameter in a model will be used to identify the likelihood that particular input values will occur when a Monte Carlo analysis is applied. The shape of PDFs can greatly affect the outcome of a Monte Carlo analysis and must, therefore, be selected with care. Because of the potential for arriving at incorrect conclusions if an inappropriate PDF is used, regulators typically require thorough documentation of the basis for selecting PDFs in the work plan and in the baseline ERA.

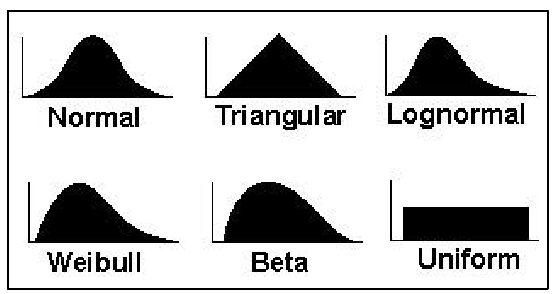

Figure 2. Types of probability density functions. Each probability density function represents the probability of occurrence (y-axis) for different values (x-axis) of a variable.

How Does Monte Carlo Analysis Work?

Overall, the concept behind applying a Monte Carlo analysis to a model is relatively simple. In a deterministic model, a single value for each of the model's input parameters is used to calculate a single output parameter. To conduct probabilistic modeling using Monte Carlo analysis each of the input parameters is assigned a distribution (PDF or PMF, as appropriate; see previous section). The output from the model is calculated many times, randomly selecting a new value from the probability distributions for each of the input parameters each time. The outputs from each run of the model are saved and a probability distribution for the output values is generated. This allows the probability of the occurrence of any particular value or range of values for the output to be calculated. Figure 3 presents a diagrammatic representation of how Monte Carlo analysis is conducted. Specific considerations for the major steps in a Monte Carlo analysis are presented in the following sections.

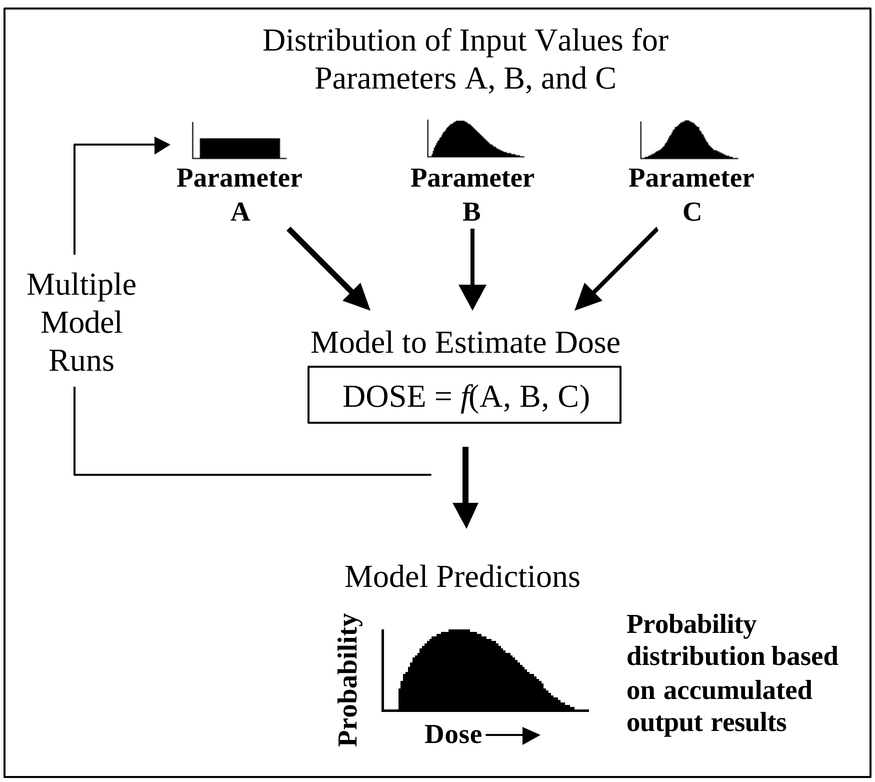

Figure 3. Diagrammatic representation of the application of Monte Carlo analysis to a model.

Defining the Statistical Distributions of Input Parameters

Defining the statistical distributions (PDFs) that will be used for the model's input parameters is probably the most challenging aspect of a Monte Carlo analysis as this is the step with the most uncertainty. It is often tempting to make assumptions about the distribution of particular input parameters when insufficient information is available to reliably determine what the actual distribution is. However, as mentioned previously, the shape of the probability distribution can greatly affect the outcome of the Monte Carlo analysis and it is extremely important that an appropriate distribution be selected. For example consider the potential differences that could result if the inputs to a model were distributed according to a normal distribution, where the occurrence of values nearer the mean will be more common than the occurrence of values farther way from the mean, versus a uniform distribution where there is an equal probability of occurrence for all values of the parameter. (Refer to Figure 2 to see the differences between these two distribution types.) In many cases the conclusions can differ greatly if different distributions for the input parameters are used.

Determining the PDF for a particular parameter typically requires the collection of a fairly large amount of sample data, unless there is already a supportable PDF (or the data to determine and generate an appropriate PDF) that can be gleaned from existing studies. Figure 4 shows a frequency distribution for fish lengths based upon samples taken at a hypothetical site. The data used to generate such a figure might be used as the basis for selecting a PDF that identifies the expected proportion of fish for each size interval in the fish population exposed to contaminants at a site. As with any exercise to

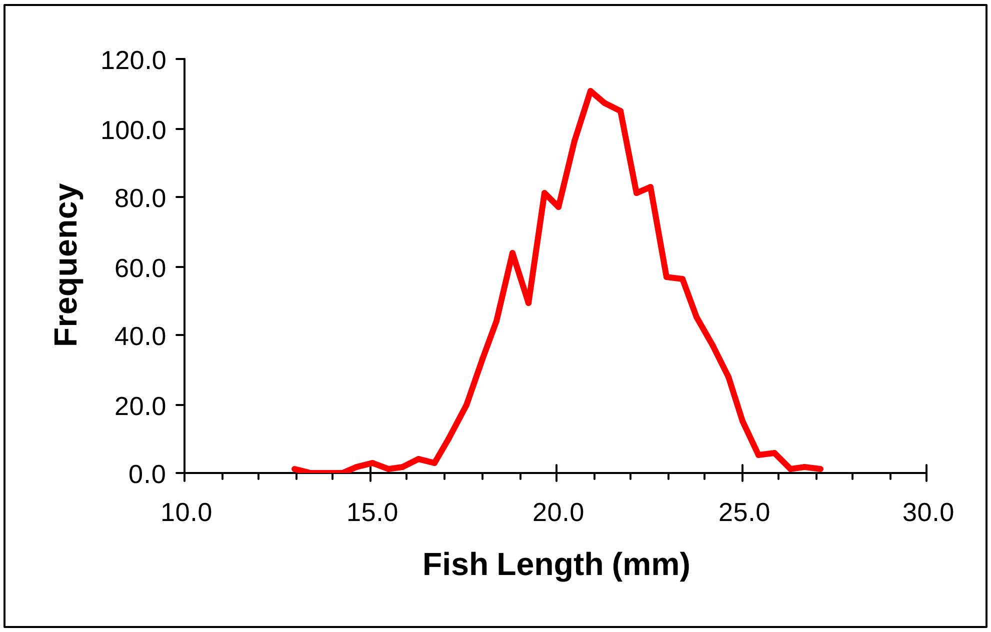

Figure 4. Frequency of occurrence for fish lengths based upon a sample.

reduce uncertainty and better characterize variability, the larger the sample size, the better the selection of a specific PDF can be supported. Once the parameters of potential distributions that fit the data have been estimated it is necessary to evaluate the quality of the fit, and, if more than one distribution is possible, to select the "best" distribution from among the candidates. There are a number of statistical techniques that can be used to help identify the type of PDF that might represent the data, although a detailed discussion of such techniques is beyond the scope of this paper. Unfortunately, in many cases there is no unambiguous measure of what constitutes the "best" fit and the risk assessor (ideally in conjunction with a statistician) must ultimately judge whether or not the fit is acceptable. Additional information pertaining to the selection of input distributions for Monte Carlo analyses can be found in a report on the proceedings of a workshop convened by the EPA in 1999 (EPA 1999). Although the focus of that document (as with most EPA documents pertaining to Monte Carlo analysis) is on human health risk assessments, many of the principles and methods discussed are pertinent to ERA as well.

Finally, it should be noted that Monte Carlo analysis does not require that PDFs be defined for all input parameters. In multiple-parameter models where there is no basis for assigning a PDF to particular parameters, it is acceptable to keep a fixed value for those parameters while assigning PDFs to parameters where sufficient information is available. In fact, identifying PDFs for all the parameters in an ERA model could be prohibitively expensive and time-consuming.

Performing Repeated Model Simulations

Once the PDFs for the input parameters have been defined, a computerized routine is used to repeatedly run the model with input parameter values selected according to the probabilities identified in the PDFs. Typically, the model is run hundreds or thousands of times. Fortunately, this tedious operation has been greatly facilitated by the availability of a number of commercially available computer programs that either operate as stand-alone programs or as add-ons to spreadsheet programs.

Analyzing the Output from the Monte Carlo Analysis

After each run of the model has been completed, the output value is saved. After all the simulations have been completed, the frequency with which particular output values were obtained is analyzed. The resulting set of output values can be evaluated to determine descriptive statistics such as the mean, range, standard deviation, etc. In addition, it is possible to evaluate the probability that the outcome will exceed a particular value or will fall within a certain range of values. For example, if the model calculates a hazard quotient (HQ) for each run, the outcome of a Monte Carlo analysis will allow a determination of the probability that the HQ will exceed a value of 1 or that the HQ will be below a particular value.

It is usually easiest to examine the output from a Monte Carlo analysis in a graphical format and most of the commercially available software packages for conducting Monte Carlo analysis provide options for graphical output. An example of a hypothetical probability distribution output from a Monte Carlo analysis for a model to estimate the HQ from exposure to a contaminant is provided in Figure 5. The figure shows the probability that particular narrow ranges of HQ values would result from exposure to the contaminant. Thus, the estimated probability that an HQ of 3.6 (the mean

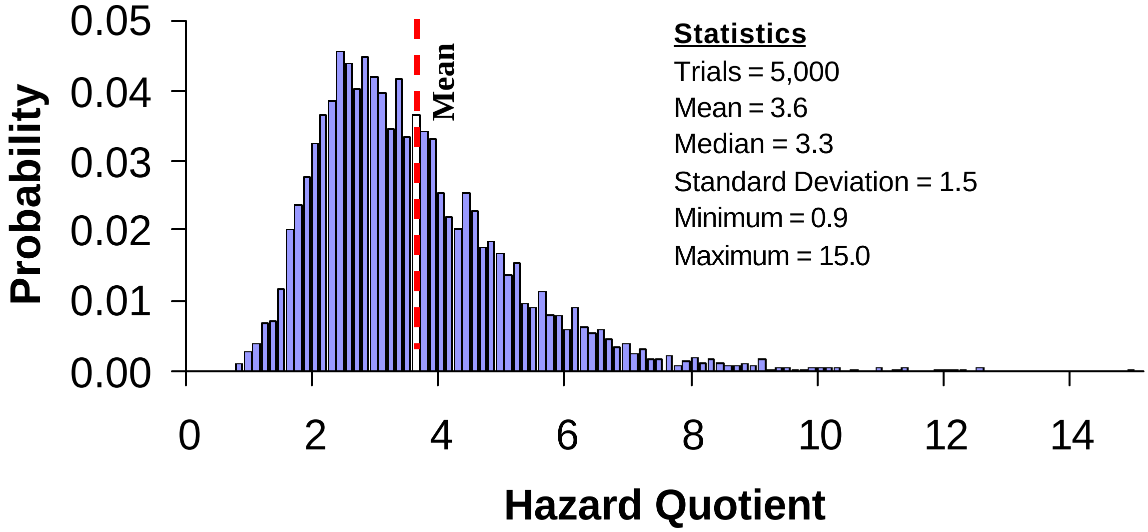

Figure 5. Hypothetical probability distribution of output from a Monte Carlo analysis, showing the estimated probability with which hazard quotient values would result from exposure to site contaminants.

value) would result from exposure to site contaminants is approximately 0.037 or 3.7%. An alternate type of graphical representation of the output, using the same results represented in Figure 5, is shown in Figure 6. This type of graph, known as a cumulative probability distribution, shows the probability that the HQ estimated by the model will be less than or equal to a specified value. Thus, Figure 6 indicates that the probability that the HQ value resulting from exposure will be less than or equal to 3.6 (the mean value) is approximately 0.61 or 61%. Such information may be useful to a risk managers, especially when compared to the deterministic results that are required in ERAs or when weighing the benefits (e.g., risk reduction) of a remedial action against costs. With appropriate explanations, the results of a Monte Carlo analysis may also be used to help interested parties, such as the public or regulators, understand the basis for risk management decisions.

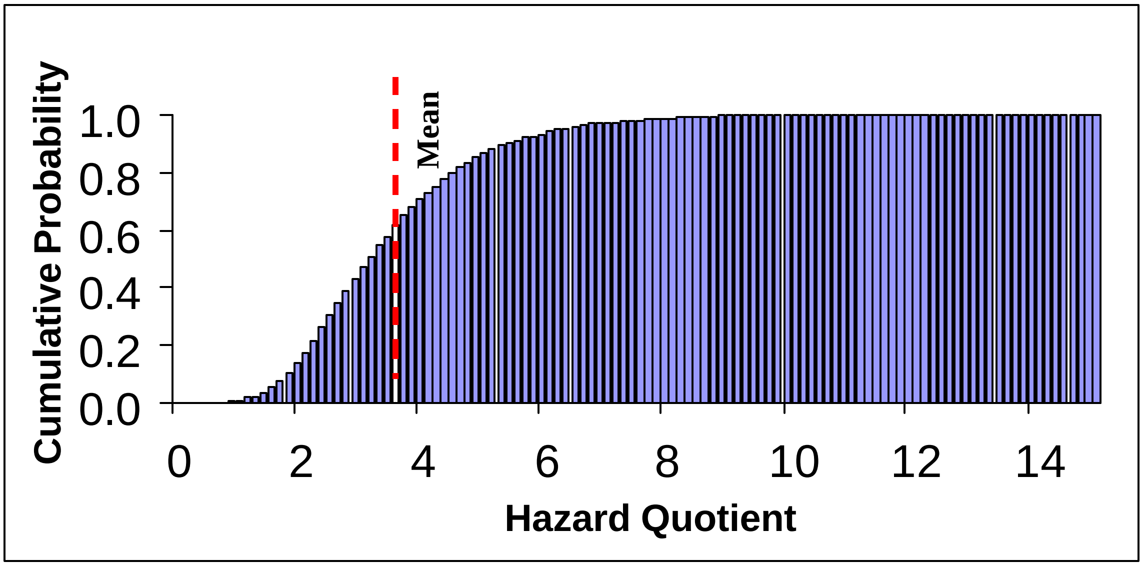

Figure 6. Hypothetical cumulative probability distribution of output from a Monte Carlo analysis, showing the probability that hazard quotient values would be equal to or lower than specific levels.

Another potential use of Monte Carlo analysis is for examining the sensitivity of a model to changes in specific parameters about which there is a high degree of uncertainty. To do this, the values of all input parameters in the model, except one, are held as fixed values. By allowing the single remaining parameter to vary in a Monte Carlo analysis, the effect of different values of that parameter on the outcome of the model can be examined. This can provide information to risk assessors and risk managers when they are deciding about the need to collect additional site-specific information by focusing attention on reducing uncertainty for parameters that will most affect the outcome (and, potentially, remedial decisions pertaining to a site).

When Should Monte Carlo Analysis Be Used In An ERA?

There is no regulatory requirement to use Monte Carlo analyses in an ERA. Thus, the decision to utilize a Monte Carlo (or other probabilistic) analysis will need to be determined on a case-by-case basis, depending upon financial, time, and personnel constraints. The use of a Monte Carlo analysis in an ERA will probably require a substantial amount of additional documentation in the project work plan and in the baseline ERA itself. There are many risk assessments for which Monte Carlo analysis would clearly be unnecessary. This is especially true for ERAs that have little need for a quantitative characterization of variability and uncertainty. For example, it would be unnecessary to conduct a Monte Carlo analysis for an ERA if the screening calculations show exposures or risks to be below levels of concern (especially if conservative protective assumptions were used to estimate input parameter values). Further, since there is both a financial and time cost associated with conducting a Monte Carlo analysis, it may be counterproductive to perform such an analysis for sites where the estimated remediation costs are low.

On the other hand, there will be situations where a probabilistic approach may have a great deal of value. For example, if the estimated cost of remediation is high, conservative terms were used for deterministic modeling, and marginal risks were identified for many of the contaminants, a Monte Carlo analysis may be warranted. There may also be times where other evidence (e.g., biological surveys and toxicity testing) indicate that the effects to biota will probably be localized and the use of a Monte Carlo approach can help evaluate the likelihood of negative site-wide effects. Before deciding to utilize a Monte Carlo approach, it is important to consider the type and amount of data that will have to be collected. Adequately defining the PDF for a particular input parameter may require a considerable amount of data collection and the sampling design may need to be adjusted to obtain appropriate information. Before committing to a Monte Carlo approach, consult with an environmental statistician to help identify data needs. Ultimately, whether or not a Monte Carlo analysis should be conducted is a matter of judgement, based upon consideration of the intended use, the importance of the ERA, and the value and insights it might provide to the risk assessor, risk manager, and other affected individuals or groups.

Regulatory Considerations

The importance of adequately characterizing variability and uncertainty in risk assessments has been emphasized in several science and policy documents issued by the EPA including the *Exposure Assessment Guidelines* (EPA 1992) , the *Policy for Risk Characterization* (EPA 1995), the *Ecological Risk Assessment Guidance for Superfund* (EPA 1997a), and the *Proposed Guidelines for Ecological Risk Assessment* (EPA 1998). In a policy statement on the use of probabilistic analysis in risk assessments, EPA (1997b) stated:

> "It is the policy of the U.S. Environmental Protection Agency that such probabilistic analysis techniques as Monte Carlo analysis, given adequate supporting data and credible assumptions, can be viable statistical tools for analyzing variability and uncertainty in risk assessments. As such, and provided that the conditions described below are met, risk assessments using Monte Carlo analysis or other probabilistic techniques will be evaluated and utilized in a manner that is consistent with other risk assessments submitted to the Agency for review or consideration. It is not the intent of this policy to recommend that probabilistic analysis be conducted for all risk assessments supporting risk management decisions.

> Such analysis should be a part of a tiered approach to risk assessment that progresses from simpler (e.g., deterministic) to more complex (e.g., probabilistic) analyses as the risk management situation requires. Use of Monte Carlo analysis or other such techniques in risk assessments shall not be cause, *per se*, for rejection of the risk assessment by the Agency. For human health risk assessments, the application of Monte Carlo and other probabilistic techniques has been limited to exposure assessments in the majority of cases. The current policy, Conditions for Acceptance and associated guiding principles are not intended to apply to dose response evaluations for human health risk assessment until this application of probabilistic analysis has been studied further. In the case of ERA, however, this policy applies to all aspects including stressor and dose-response assessment."

The EPA has recently provided guidance on probabilistic risk assessment as part of the Risk Assessment Guidance for Superfund (EPA 2001). This guidance document provides guidance on applying probabilistic analysis to both human health and ecological assessment.

Conditions for Acceptance

In order for risk assessments incorporating probabilistic risk assessment methods (including Monte Carlo analysis) to be accepted by the EPA for review and evaluation, several conditions delineated in the EPA policy on probabilistic analysis must be met (EPA 1997b). These conditions, which are intended to promote the use of sound methods and to assist with the ability of regulators and other interested parties to evaluate and reproduce the calculation results are summarized below.

Clearly Identify the Purpose and Scope of the Monte Carlo Analysis

The purpose and scope of the assessment should be clearly articulated in the problem formulation section, including a full discussion of any highly exposed or highly susceptible subpopulations that will be evaluated. Discuss the questions the assessment is meant to address and clearly define all assessment endpoints.

Fully Document the Methods for the Analysis

As discussed in previous sections, the methods used for the analysis (including models used, the data upon which the analysis is based, and assumptions pertaining to the PDFs) can have a significant impact upon the results. Consequently, it will be extremely important to document the analysis fully. Such documentation should be easily located in the report and should include a discussion of the degree to which the data used are representative of the population under study. Be sure to clearly identify the models and software used to generate the analysis. Regulators will require sufficient information so that they can independently reproduce the results of the analysis.

Provide a Sensitivity Analysis for All Models

A sensitivity analysis is used to determine the overall effect that a change in the value for each input variable has on the outcome of a model. This is typically accomplished by varying the values for a single input parameter across a range of values while all other input parameters are held constant. Subsequently, the strength of the relationship between each input parameter and the model output can be evaluated. In this manner, it can be determined which input parameters are of the greatest importance to the results. The results of sensitivity analyses must be presented and discussed in the ERA. It will be in your best interest to simplify the Monte Carlo analysis by using the results of a sensitivity analysis to focus the Monte Carlo analysis on compounds, pathways, and factors of importance to the ERA, as this will reduce the time and cost for the analysis.

Consider Correlation Among Input Variables

Correlation among input parameters used in a Monte Carlo analysis can have substantial effects upon the results in some cases. This is an area where a qualified statistician can provide valuable assistance. Because many of the commercial packages that are available for conducting Monte Carlo analysis allow correlation to be taken into account, there are ways to evaluate the effects of dependencies between the input variables. Such an evaluation should be conducted and presented in the ERA.

Present Complete Information for All Input and Output PDFs

Information for each input and output distribution will need to be provided in the ERA. Include tabular and graphical representations of the distributions that indicate the location of any point estimates of interest (e.g., mean, median, 95th percentile). The selection of input distributions must be clearly explained and justified.

Include Deterministic Results

The deterministic calculations of exposures and risks based on point estimates must be included in the ERA. Providing these values will allow comparisons between the Monte Carlo analysis and the deterministic assessments. Deterministic estimates may more clearly address specific questions and may facilitate risk communication. When comparisons are made, it is important to explain the similarities and differences in the underlying data, assumptions, and models.

Above all, it is extremely important that concurrence be reached with regulators prior to undertaking a Monte Carlo analysis. The proper place to identify the specific methods to be used and the models that Monte Carlo analysis will be applied to is in the work plan for the ERA. Getting agreement on methods and parameters before using them in the analysis will help prevent situations where time and money are spent on conducting a Monte Carlo analysis that is unacceptable to the regulators and cannot be presented in the final ERA.

Conclusion

Monte Carlo is potentially a powerful tool for examining the effects of variability and uncertainty on the outcome of modeling calculations used in ERAs. It is capable of providing information to risk managers about the probability that particular outcomes will result from contamination levels present at a site. Although the regulatory community has developed guidance pertaining to the use of Monte Carlo analysis in ERAs, few ERAs to date have incorporated Monte Carlo analysis. There are a number of considerations to be made before undertaking Monte Carlo analyses for an ERA, especially the amount of data that will be required to adequately determine the appropriate PDFs for input parameters to models. Remedial project managers desiring to incorporate Monte Carlo analyses into an ERA should utilize personnel with appropriate expertise, including environmental statisticians, to help identify the data needs as early in the ERA process as possible. In addition, regulators need to be consulted and agreements need to be obtained prior to initiating the use of Monte Carlo analyses in specific ERAs.

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Acronyms

ERA — ecological risk assessment
EPA — Environmental Protection Agency
HQ — hazard quotient
PDF — probability density function
PMF — probability mass function

Glossary

Correlation — A measure of the statistical association among random variables.

Deterministic Risk Assessment — A risk assessment in which the population and environmental parameters are assumed to be constant.

Ecological Risk Assessment — The process that evaluates the likelihood that adverse ecological effects may occur or are occurring as a result of exposure to one or more stressors.

Hazard Quotient — The ratio of an exposure level to a substance to a toxicity value selected for the risk assessment for that substance.

Human Health Risk Assessment — The process that evaluates the likelihood that adverse human health effects may occur as the result of exposure to one or more hazardous substances.

Monte Carlo Analysis — A computer-based method of analysis developed in the 1940s that uses statistical sampling techniques in obtaining a probabilistic approximation to the solution of a mathematical equation or model.

Probabilistic Risk Assessment — A risk assessment that uses methods such as Monte Carlo Analysis, to quantify the probability of a risk.

Probability Density Function — A function that expresses the probability that an observation of a continuous variable (a variable that can assume any value within a defined range) will fall within some very small interval. May alternatively be referred to in the literature as a probability function or frequency function.

Probability Mass Function — A function that expresses the probability that a discrete variable (a variable that can only assumed certain isolated or fixed values) will take on a specific value.

Uncertainty — Imperfect knowledge about the present or future state of specific factors, parameters, or models.

Variability — Observed differences attributable to true heterogeneity or diversity in a population or exposure parameter.

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