Uncertainty Modeling and Analysis in Civil Engineering

edited by **Bilal M. Ayyub**

CRC Press
Boca Raton Boston London New York Washington, D.C.

21. Quantitative Analysis of Variability and Uncertainty in Energy and Environmental Systems

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1. INTRODUCTION

The quantification of variability and uncertainty in energy and environmental systems is receiving increasing attention. The ability to propagate random variables through computer-based models has been enhanced by the development of efficient numerical simulation methods combined with the availability of low cost, powerful personal computers. Add-in packages for standard spreadsheets, such as @Risk* and Crystal Ball,† are readily available and allow anyone with a personal computer to do probabilistic analysis. As many of the computational challenges to probabilistic analysis have been removed, the philosophical and conceptual aspects are more clearly in focus. For example, as with any type of modeling activity, a concern is that model predictions are only meaningful if both the model and model inputs are properly specified.

In this section, we address some of the broader motivations for doing probabilistic analysis. In Section 2, we present a brief discussion of methodological issues regarding probabilistic analysis. Three case studies are then presented. The first case study illustrates the application of probabilistic methods to the quantification of technological risk for energy and environmental control systems. The second case study highlights the role of probabilistic analysis in integrated assessment, with application to acid deposition. The third case study emphasizes the distinction between variability and uncertainty.

Some of the main reasons for doing probabilistic analysis are summarized as follows:

Scientific Rigor. It is a matter of good scientific practice to quantify the levels of uncertainty associated with any measurement or any model prediction. For example, characterizations of uncertainty in each measurement taken in a time series, such as for an environmental pollutant, enables comparisons of measurements to determine whether there are any significant trends in the change in pollutant concentrations with respect to time. In the absence of uncertainty characterizations, it would be unknown as to whether observed changes represent an underlying trend or if they are random artifacts of measurement errors.

Knowledge of Uncertainty Can Change Decisions. From a pragmatic and decision analytical perspective, characterization of uncertainty is important if it affects a decision. Decisions regarding

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selection of environmental control technologies, specification of control efficiencies, operation of a system of power plants, and others are better informed if uncertainties are considered. For example, the performance and cost of new process technologies is typically misestimated, especially when predictions regarding commercial-scale performance and cost are made during early stages of technology development.[1] The use of inaccurate point-estimates can lead to misallocation of resources, running into millions or billions of dollars, compared to decisions that would have been made had the risks as well as the potential payoffs of the technology options been quantified.

Targeting Research to Reduce Uncertainty. Probabilistic modeling allows the key sources of uncertainty in model inputs to be identified. Knowledge regarding the key sources of uncertainty can be used to target data collection or research to reduce key uncertainties. By targeting research activities in this manner, research will be prioritized to areas that will have the most significant effect on reducing uncertainties in model predictions, such as for the performance and cost of environmental control technologies or the predictions of ambient pollutant concentrations or human exposures. Conversely, probabilistic analysis can be used to identify model inputs that have no significant effect on an answer, even though they may be subject to uncertainty. In many cases, even for models with dozens or hundreds of uncertain inputs, it is typically only a handful that contribute most to uncertainty in the model output. Thus, it is possible to reduce by orders-of-magnitude the amount of data collection or research needed to most effectively improve the precision of predictions.

There are also situations in which probabilistic analysis may not be needed. For example, suppose that we are interested in determining whether or not a chemical in the ambient air poses a significant health risk to an exposed population. There are simple models that can be used, in combination with highly conservative default assumptions, to make a preliminary estimate regarding whether the risk to the population may be above levels of regulatory or health concern. These types of analyses produce a point estimate that is believed to be protective of maximally exposed individuals who may be highly susceptible to adverse effects. However, in this type of point estimate upper bound (or screening) analysis, it is unknown as to what percentage of the population would be "protected." However, it is intended that it would be highly unlikely for any real person to have a risk higher than the hypothetical person considered in the point estimate. Thus, if this type of upper bound analysis indicates that risks are below some *de minimus* level, then it is not necessary to pursue any further action, either in terms of additional analysis or corrective action. However, if the upper bound level is above the *de minimus* level, then it is unknown as to whether any real people would be subject to a significant risk. In this case, a probabilistic analysis, in which the variation in exposures to different members of the population is considered, would be needed to provide insight into whether corrective action is truly needed. A probabilistic analysis would provide information regarding the levels of exposure and risk to different members of the population. Policy decisions could then be made based upon protecting a specified percentage of the population against a particular level of risk. In fact, current guidance from the U.S. Environmental Protection Agency has recommended that exposures to high-end individuals, who are at or above the 90th percentile of the population in terms of exposures, be considered in risk assessments.[2]

2. OVERVIEW OF PROBABILISTIC METHODS

In this section, we provide an overview of the main considerations and features of probabilistic analysis. Many of these are illustrated in the case studies of the following sections.

2.1 PHILOSOPHY OF UNCERTAINTY ANALYSIS

The "classical" approach in probability theory requires that estimates for probability distributions must be based on empirical data. However, in many practical cases, the available data may not be relevant to the problem at hand, or there may be few data points to support a statistical analysis. Thus, statistical manipulation of data may be an insufficient basis for estimating uncertainty in a real system of interest. As a result, some degree of judgment about the available data may be required. Furthermore, even the application of statistical techniques, such as goodness-of-fit (GOF) tests, requires considerable judgment. For example, the analyst makes judgments about what types of parametric distributions are appropriate to represent uncertainty in a given empirical quantity.

An alternative approach differs in how probability distributions are interpreted. In the so-called "Bayesian" view, the assessment of the probability of an outcome is based on a "degree of belief" that the outcome will occur, based on all of the relevant information an analyst currently has about the system. Thus, the probability distribution may be based on empirical data and/or other considerations, such as technically informed judgments or predictions. People with different information or theoretical beliefs may estimate different distributions for the same variable.[3] The assessment of uncertainties requires one to think about all possible outcomes and their likelihood, not just the "most likely" outcome.

2.2 A TAXONOMY OF UNCERTAINTY AND VARIABILITY

There are a number of distinct sources of uncertainty in analyses of energy and environmental problems. These come under the general headings of model or structural uncertainty and parameter uncertainty. Several authors, including Morgan and Henrion[3], Finkel[4], and others, provide more detail regarding sources of uncertainty. Sources of uncertainty are also discussed in some U.S. Environmental Protection Agency documents.[2] A few key concepts are summarized here.

2.2.1 Model Uncertainty

The structure of mathematical models employed to represent scenarios and phenomena of interest is often a key source of uncertainty, due to the fact that models are often only a simplified representation of a real-world system, and that the problem boundary encompassed by a model may be incomplete or incorrect. Significant approximations are often an inherent part of the assumptions upon which a model is built. Competing models may be available based on different scientific or technical assumptions. Furthermore, the limited spatial or temporal resolution (e.g., grid size) of many models is also a type of approximation that introduces uncertainty into model results. Different sources of model uncertainties, and how they may be evaluated, are summarized by Frey[5].

2.2.2 Parameter Uncertainty

Morgan and Henrion have identified a number of different types of quantities used in models.[3] These include:

- *Empirical:* Measurable, at least in principle (e.g., pollutant concentration).
- *Defined constants:* Some quantities whose values are accepted by convention, such as Planck's constant or the speed of light, are actually empirical quantities subject to measurement error, albeit small.
- *Decision variables:* These are parameters over which a decision maker exercises control, such as the maximum acceptable emission rate for a given emission source. Thus, it is not appropriate to treat this quantity probabilistically. Rather, the sensitivity of the result to different values of the decision variable(s) should be explored using sensitivity analysis.
- *Value parameters:* These represent the preferences or value judgments of a decision maker. Examples include the discount rate and parameters of utility functions used in decision analysis.
- *Model domain parameters:* These are parameters that are associated with a model, but not directly with the phenomenon the model represents. For example, the spatial or temporal grid size is a model domain parameter introduced in numerical models.

Of the types of quantities identified above, only empirical quantities are unambiguously subjected to uncertainty. The other types of parameters represent quantities which are almost always more properly treated as point-estimates reflecting convention, the explicit preferences of a decision maker (broadly defined), or a discrete quantity by its nature (e.g., grid size). Thus, we focus here on identifying sources of uncertainty in empirical quantities. These include:

- *Random error and statistical variation:* This type of uncertainty is associated with imperfections in measurement techniques. Statistical analysis of test data is thus one method for developing a representation of uncertainty in a variable.
- *Systematic error:* The mean value of a measured quantity may not converge to the "true" mean value because of biases in measurements and procedures.
- *Variability:* Some quantities are variable over time, space, or some population of individuals (broadly defined) rather than for any individual event or component.
- *Inherent randomness or unpredictability:* Some quantities may be irreducibly random even in principle, the most obvious example being Heisenberg's Uncertainty Principle. However, this concept is often applied to quantities that are in principle measurable precisely but as a practical matter (due to cost, for example) are not.
- *Lack of empirical basis:* Lack of experience about or knowledge of a process or system is a source of uncertainty. This type of uncertainty cannot be treated statistically, because it requires predictions about something that has yet to be built, tested, or measured.

2.2.3 Variability and Uncertainty

In many environmental problems, the distinction between variability and uncertainty is critically important. Variability is a heterogeneity between individual members of a population of some type. In principle, the characteristics of a specific member of a population are knowable with certainty. Thus, the frequency distribution for the population reflects true differences between individuals. Knowing the frequency distribution for variability in the population can aid in determining whether the population should be disaggregated into smaller groups that are more nearly homogeneous. This type of information is important, for example, in identifying subgroups especially susceptible to specific health risks from exposures to a given chemical.

However, there may be uncertainty in the characteristics of specific members of the population, due to measurement error or other sources of uncertainty as described above. In these cases, there is a resulting uncertainty about the variability frequency distribution. For example, while individuals may be known to have different exposure levels to a certain pollutant, their health effects may be uncertain due to the limited applicability of dose-response models extrapolated from animal bioassay test results. Thus, the population distribution for health effects (e.g., excess cancers) may be both variable and uncertain.

To complicate matters further, however, it is possible for variability to be interpreted as uncertainty under certain conditions. For example, suppose we are interested in the exposure level faced by an individual selected at random from a population. If we select an individual at random, the probability of selecting an individual with a given exposure is the same as the relative frequency of all individuals in the population subject to the given exposure. Hence, in this case variability represents an *a priori* probability distribution for the exposure faced by a randomly selected individual. However, except for this special case, there is always a distinction between variability and uncertainty.

Variability and uncertainty are referred to by a variety of terms depending on the background of particular investigators. For example, variability is sometimes referred to as aleatory uncertainty, stochastic variability, and interindividual variability. Uncertainty has been referred to as fundamental or epistemic uncertainty.[6-9] Here, we use the term *probabilistic analysis* to be inclusive of quantitative analysis of either variability and/or uncertainty.

Both variability and uncertainty may be quantified using probability distributions. However, the interpretation of the distributions differs in the two cases. Similar to other authors, the terminology employed here is to consider that distributions for variability represent the relative frequency with which members of a population may have values of a quantity within some specified range. Thus, distributions for variability are referred to here as *frequency distributions*. In contrast, uncertainty regarding a quantity implies that there is some range of possible values for a quantity, and that based upon data analysis or expert judgment one can specify the probability, or degree of belief, that the true value of the quantity will be within a specified range. Thus, distributions for uncertainty are referred to here as *probability distributions*. To some, this distinction appears to be semantic. However, it is useful to have a language with which to denote distinctions in the representation of variable versus uncertain quantities.

2.3 DEPENDENCE AND CORRELATION

A question that arises in the early stages of developing a simulation of uncertainty and variability is whether there is dependence between input variables to a model. In many cases there is, due to the use of simplified models. In a complete model, the sources of dependence between inputs would be explicitly modeled. In a simplified model, some quantities that may be more properly modeled as state variables are treated as if they are input (exogenous) variables. Thus, it may be necessary to approximate the dependence between input variables. For example, in a simplified process model, temperature and chemical reaction conversion rate may both be treated as input variables, whereas in reality the chemical reaction conversion rate is a function of temperature.

There are several approaches to dealing with dependence. These include: explicit modeling of the dependence; parameterization; stratification; bootstrap simulation; and simulation of correlations. Each of these approaches is briefly discussed.

Modeling dependence explicitly involves the development of a more detailed model which captures the source of dependence between two quantities. Thus, in the previous example, a chemical kinetic reaction model in which reaction rate is a function of temperature would capture the dependence between temperature and conversion rate. Such a model formulation would also change conversion rate from an input variable to a model state variable.

Parameterization refers to grouping the input variables and treating the grouping as a new input variable. This treatment of dependence is useful when there is linear dependence between the variables. For example, air inhalation rate and body weight may both be variables in an exposure model. The inhalation rate is at least partly dependent on body weight. Thus, a new parameter, inhalation rate divided by body weight, may be used to capture at least some of the dependence between the two.

Rather than try to model dependence, another approach attempts to reduce the effects of dependence. This approach, stratification, involves subdividing the problem by creating several subgroups or strata. For example, if the problem features a population of individuals with widely varying body weights and inhalation rates, the problem could be subdivided by body weight. Thus, there would be less variance in inhalation rate within the body weight subgroups. As a result, the effect of correlation or dependence within the strata would be smaller than for the population as a whole.

Bootstrap simulation can be used to capture nonlinear and even nonmonotonic dependencies for the sampling distributions of the parameters of frequency distributions. The sampling distributions, such as for the mean and variance of a normal distribution, represent uncertainty due to random sampling error. This topic is discussed in more detail in the section on Case Study 3. A given mean and variance specifies one possible frequency distribution, which in turn represents variability in the quantity of interest. Thus, bootstrap simulation can be used to distinguish between variability and uncertainty to capture dependencies between the uncertain parameters of frequency distributions for variability. Frey and Rhodes present an example.[10] Resampling techniques can also be used to simulate values from an actual data set, rather than to make assumptions regarding an underlying parametric probability distribution.

Correlations between distributions may be simulated using numerical methods. For example, there are easily applied techniques for inducing correlations between normal distributions in Monte Carlo simulations.[3] There are more generalized techniques for inducing rank correlations among multiple variables.[11]

In the absence of sufficient data from which to characterize correlations, there are alternative approaches. One is to try to estimate the actual correlations through some type of expert elicitation process. However, it is generally more difficult to estimate correlation coefficients or covariance matrices than it is to make judgments about probability or frequency distributions.[3] Another approach is to employ a generalized rank ordering pairing technique to explore the sensitivity of modeling results to alternative assumptions about correlations. In such an approach, high or low correlations may be compared to see what effect, if any, there is on model results.

Correlations among input variables to a model may have little effect on modeling results in several cases. If all of the correlated random variables do not contribute significantly to uncertainty in key model outputs of interest, then correlations among them will tend to have little effect on model results. When only one of two or more statistically dependent input variables contributes significantly to uncertainty in a model result, correlations will also have little effect on the result. The importance of the correlation also depends upon the structure of the model and the output of interest. Nonlinear models, depending on their features, may tend to magnify or reduce the effects of uncertainties in selected inputs. Correlations in inputs will typically have a more pronounced effect on the tails of the model output distribution than on the central values.

2.4 ENCODING UNCERTAINTIES AS PROBABILITY DISTRIBUTIONS

There are two fundamental approaches for encoding probability distributions. These include statistical estimation techniques and expert judgments. A combination of both methods may be appropriate in many practical situations. For example, a statistical analysis of measured test data may be a starting point for thinking about uncertainties in a hypothetical commercial-scale system for a new process technology. One must then consider the effect that systematic errors, variability, or uncertainties about scaling-up the process might have on interpreting test results for commercial scale design applications.[12]

2.4.1 Statistical Techniques

Statistical analysis is an inherently subjective activity. It involves making decisions regarding which types of statistical estimators to use, what types of probability models to consider, what types of statistical tests to use, and what confidence levels to assume. The results of statistical analyses may be inconclusive. For example, if one wishes to fit a parametric distribution to a dataset, then one must consider how to: (1) choose candidate probability distributions (e.g., based upon knowledge of processes that created the data; by inspection of the central moments of the data set and comparison to moment planes for distributional families); (2) estimate the parameters of the distribution (e.g., method of moments, maximum likelihood, probability plots); (3) evaluate the goodness of fit of the distribution (e.g., probability plots, regression techniques, statistical tests); (4) choose a significance level (e.g., 0.1, 0.05, 0.025, 0.01, 0.005); and (5) interpret the results, especially when these methods cannot be used to find a unique answer. For example, if several statistical tests indicate that, for a given data set, neither a normal nor a lognormal distribution can be rejected as a possible fit to the data, then it is up to the analyst to make a final judgment. In reality, it is possible that neither of these options is the "correct" one. For these reasons, many authors stress that statistical analysis involves a significant amount of judgment.[13,14] Case Study 3 provides an example of data analysis.

Nonrepresentative data pose a difficult challenge for analysts. This is because statistical methods are not a sufficient basis for quantifying uncertainty in such cases. For example, it is only possible to evaluate systematic errors in a measured data set quantitatively if the "true" value of the quantity being measured is known. Thus, in the absence of a known datum, expert judgment may be

required to adjust the results of a statistical analysis to account for potential sources of bias. In addition, a nonrepresentative sample may place too much weight on a subpopulation of interest. For example, if we are interested in characterizing fish intake as part of an assessment of exposures to food-borne contaminants, and if we only considered the consumption of fish purchased in supermarkets, we would underrepresent a portion of the population that might include subsistence fishermen. Thus, it might be appropriate to adjust the upper bound of the observed data set if there is some information available regarding the nature of underrepresented subpopulations. This type of adjustment, while intended to represent variability, is highly uncertain because it is not fully supported by empirical observations.

2.4.2 Judgments about Uncertainties Using Expert Elicitation

In this section, we consider the situation in which insufficient data are available to merit the use of classical statistical techniques to construct probabilistic representations of model inputs. This may be the case when there are few data points, or when the available data are not representative of the quantity of interest. In making judgments about a probability distribution for a quantity, there are a number of approaches (heuristics) that people use which psychologists have observed. Some of these can lead to biases in the probability estimate. Three of the most common are briefly summarized.[3]

1. *Availability.* The probability that experts assign to a particular possible outcome may be linked to the ease (availability) with which they can recall past instances of the outcome.
2. *Representativeness* has also been termed the "law of small numbers." People may tend to assume that the behavior they observe in a small set of data must be representative of the behavior of the system, which may not be completely characterized until substantially more data are collected.
3. *Anchoring and adjustment* involves using a natural starting point as the basis for making adjustments. For example, an expert might choose to start with a central "best guess" value. However, the adjustment from the central value to the extreme values is often insufficient, with the result that the probability distribution is too tight. This phenomena is *overconfidence*, because the expert's judgment reflects less uncertainty in the variable than it should.

Judgments also may be biased for other reasons. One common concern is *motivational bias*. This bias may occur for reasons such as: (a) a person may want to influence a decision to go a certain way; (b) the person may perceive that they will be evaluated based on the outcome and might tend to be conservative in their estimates; (c) the person may want to suppress uncertainty that they actually believe is present in order to appear knowledgeable or authoritative; and (d) the expert has taken a strong stand in the past and does not want to appear to contradict themself by producing a distribution that lends credence to alternative views.[3]

2.4.3 Designing an Elicitation Protocol

From studies of how well calibrated judgments about uncertainty are, it appears that the most frequent problem encountered is overconfidence. Knowledge about how most people make judgments about probability distributions can be used to design a procedure for eliciting these judgments. Examples of elicitation methods are given elsewhere.[3,15-21] Elicitation protocols typically have five to ten major steps and the elicitation process may require several hours to a full day. The appropriate procedure depends on the background of the expert and the quantity for which the judgment is being elicited. For example, if an expert has some prior knowledge about the shape of the distribution for the quantity, then it may be appropriate to ask him/her to think about extreme values of the distribution and then to draw the distribution. On the other hand, if an expert has little statistical background, it may be more appropriate to ask him/her a series of questions. For example, the expert might be asked the probability of obtaining a value less than or equal to some value x, and then the question would be repeated for a few other values of x. The judgment can then be graphed by an elicitor, who would review the results of the elicitation with the expert to see if he/she is comfortable with the answers.

To overcome the typical problem of overconfidence, it is usual to begin by thinking about extreme high or low values before asking about central values of the distribution. In general, experts' judgments about uncertainties tend to improve when: (1) the expert is forced to consider how things could turn out differently than expected (e.g., high and low extremes); and (2) the expert is asked to list reasons for obtaining various outcomes.

2.5 PROBABILISTIC MODELING

In order to analyze uncertainties, a probabilistic modeling environment is required. In some cases, either exact or approximate analytical solutions may be appropriate.[3,13-15] However, numerical methods can be used with a larger variety of problems. A typical approach is the use of Monte Carlo simulation.[3,13,22] In Monte Carlo simulation, a model is run repeatedly, using different values for each of the uncertain input parameters each time. The values of each of the uncertain input parameters are generated based on the probability distribution for the parameter. If there are two or more uncertain input parameters, one value from each is sampled simultaneously in each repetition in the simulation. Over the course of a simulation, perhaps 20, 50, 100, or even more repetitions may be made. The result is a set of sample values for each of the model output variables, which can be treated statistically as if they were an experimentally or empirical observed set of data.

Although the generation of sample values for model input parameters is probabilistic, the execution of the model for a given set of samples in a repetition is deterministic. The advantage of Monte Carlo methods, however, is that these deterministic simulations are repeated in a manner that yields important insights into the sensitivity of the model to variations in the input parameters, as well as into the likelihood of obtaining any particular outcome. Monte Carlo methods also allow the modeler to use any type of probability distribution for which values can be generated on a computer, rather than to be restricted to forms which are analytically tractable.

2.5.1 Monte Carlo Simulation

The generation of random variables using Monte Carlo simulation is done using a variety of methods. In order to illustrate the general concept behind Monte Carlo simulation, we briefly describe one of these, which involves the use of the inverse cumulative distribution function (cdf) of a probability distribution. A more detailed discussion can be found in Ang and Tang[22]. In random Monte Carlo simulation, a pseudo-random number generator is used to generate uniformly distributed numbers between 0 and 1 for each uncertain variable. The sample values for the random variables are calculated using the inverse cdf functions based on the randomly generated fractiles.

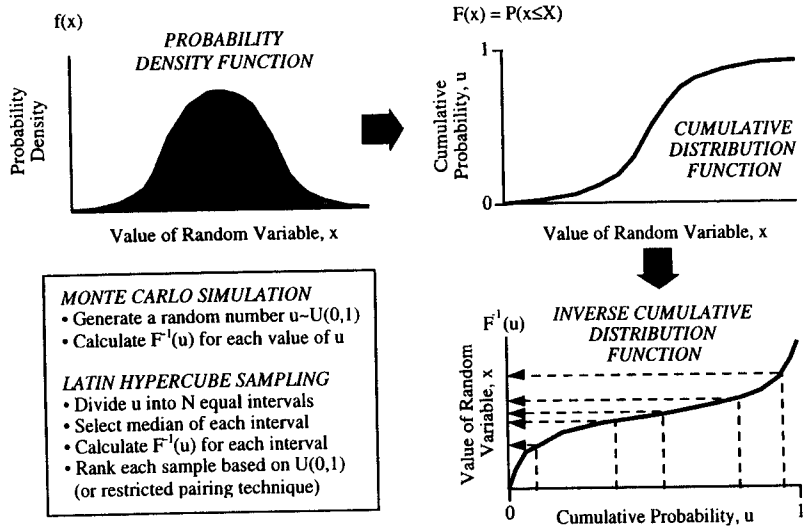

Figure 1. Monte Carlo Simulation.

This approach is shown schematically in Fig. 1. Sample values are generated for each random variable in the model. For a given iteration of the model, one random value for each of the model inputs is used. A single value of the model outputs are calculated. The process is repeated until the desired number of model iterations is completed.

2.5.2 Latin Hypercube Sampling

An alternative to random Monte Carlo simulation is Latin Hypercube Sampling (LHS). In LHS methods, the fractiles that are used as inputs to the inverse cdf are not randomly generated. Instead, the probability distribution for the random variable of interest is first divided into ranges of equal probability, and one sample is taken without replacement from each equal probability range. However, the ranking (order) of the samples is random over the course of the simulation, and the pairing of samples between two or more random input variables is usually treated as independent. In median LHS, one sample is taken from the median of each equal-probability interval, while in random LHS one sample is taken at random within each interval.[3]

LHS methods guarantee that values from the entire range of the distribution will be sampled proportional to the probability density of the distribution. Therefore, the number of samples required to adequately represent a distribution is less for LHS than for random Monte Carlo sampling. LHS is generally preferred over random Monte Carlo simulation.[3,23,24] As noted earlier, restricted pairing techniques are available for the purpose of inducing correlations between variables in LHS.[11,25]

2.5.3 Selecting Sample Size

The sample size corresponds to the number of repetitions used in the probabilistic simulation. The selection of sample size is usually constrained at the upper end by the limitations of computer software, hardware, and time, and at the lower end by the acceptable precision for model results. In cases where the analyst is most interested in the central tendency of distributions for output variables, the sample size can often be relatively small. However, in cases were the analyst is interested in low probability outcomes at the tails of model output distributions, large sample sizes may be needed. As sample size is increased, computer runtime, memory use, and disk use may become excessive. Therefore, it may be important to use no more samples than are actually needed for a particular application. Methods for selecting sample sizes for Monte Carlo simulation are described elsewhere.[3,13,22]

2.5.4 Analyzing Results

Sample correlation coefficients are a simple but useful tool for identifying the linear correlations between uncertain variables. Other techniques are available in software packages such as one developed by Iman, Shortencarier, and Johnson[26]. These output analysis techniques are described here briefly.

Partial correlation coefficients (PCC) are estimated using stepwise linear regression. The input variable most highly correlated the output variable of interest is assumed as the starting point. The partial correlation technique then searches for another input variable which is most highly correlated with the *residuals* of the regression model already containing the first input variable. The process is repeated to add more variables in the analysis. The partial correlation coefficient is a measure of the unique linear relationship between the input and dependent variables that cannot be explained by variables already included in the regression model. Standardized regression coefficients (SRC) are calculated based upon multivariate regression of an output variate based on the inputs. SRCs measure the shared contribution of the input to the output, because all of the simulation input uncertainties are included in the regression analysis simultaneously. The SRCs are analogous to the partial derivatives of the output variable with respect to each input variable.

PCC and SRC analysis is appropriate when the relationship between input and output variables is linear; however, by basing the regression analysis on the ranks of the samples for each variable, rather than on the values of the samples, the PCC and SRC techniques can be extended to nonlinear, monotonic cases. These techniques are known as partial rank correlation coefficients (PRCC) and standardized rank regression coefficients (SRRC).[26]

Both sample size and the magnitude of the coefficients must be considered in evaluating the statistical significance of PCC, SRC, PRCC, and SRRC results. Edwards provides a discussion of tests of significance for coefficients of determination and correlation coefficients.[27]

3. CASE STUDY 1: PROBABILISTIC MODELING OF ENERGY AND ENVIRONMENTAL TECHNOLOGIES

This case study focuses on the application of probabilistic methods to advanced power generation and environmental control technologies. Specifically, we focus on Integrated Gasification Combined

Cycle (IGCC) systems. IGCC systems are a promising approach for clean and efficient coal-based power generation that are capable of high thermal efficiencies and low discharges compared to conventional pulverized coal (PC) combustion-based technologies. However, there is limited commercial experience with IGCC systems, and many promising concepts have not yet been demonstrated in full-size and integrated plants.[28] A number of large-scale demonstration projects are underway.[29,30]

The uncertain nature of limited performance and cost data for first generation systems, coupled with uncertainties associated with alternative process configurations, motivates a systematic approach to evaluating the risks and potential payoffs of alternative concepts. To explicitly represent uncertainties in IGCC systems, a probabilistic modeling approach has been developed and applied. This approach features: (1) development of sufficiently detailed engineering models of performance, emissions, and cost; (2) implementation of the models in a probabilistic modeling environment; (3) development of quantitative representations of uncertainties in specific model parameters based on literature review, data analysis, and elicitation of technical judgments from experts; and (4) modeling applications for cost estimating, risk assessment, and research planning.

An advanced IGCC system featuring hot gas cleanup technology is analyzed and evaluated. This evaluation includes control of NO_x emissions from an air-blown fixed-bed gasifier-based system using selective catalytic reduction (SCR). Results will illustrate the types of insights provided by a probabilistic method for evaluating advanced process technologies.

3.1 INTEGRATED GASIFICATION COMBINED CYCLE TECHNOLOGY DESCRIPTION

The cost of conventional pulverized coal-fired power plants has tended to increase, while plant efficiency has tended to decrease, due to requirements for emission control technologies.[31] Natural gas- and oil-fired systems based on gas turbine combined cycle technology have high efficiencies, but consume expensive premium fuels. Syngas produced by coal gasification can be used to fuel a gas turbine. By integrating the steam cycle with the coal gasifier, the overall thermal efficiency can be optimized. Potential advantages of IGCC over PC power plants include higher thermal efficiency, a capability for high (over 98%) sulfur removal efficiency, lower NO_x emissions, low particulate matter emissions, reduced solid waste due to byproduct recovery of elemental sulfur, reduced cooling water requirements, reduced land requirements and a capability to burn coal, oil, or natural gas.[28]

In IGCC systems, environmental control is required not just to meet environmental regulations, but also for proper plant operation. For example, pollutants such as sulfur species and ash particles have deleterious effects on key components of IGCC systems, such as the gas turbine, and therefore must be controlled. In addition, the environmental control systems significantly affect the thermal cycle and, hence, plant efficiency. There are many variations of IGCC power plant designs, based primarily on differences in the coal gasifier technology, coal gas cleanup system, byproduct recovery options, and gas turbine technologies employed. We focus on just one of these to illustrate the application of probabilistic analysis to technology assessment.

3.2 AN EXAMPLE: LURGI GASIFIER-BASED IGCC SYSTEM

The Lurgi dry-ash coal gasification technology is the oldest of the technologies most commonly considered for IGCC systems. This process was developed in the 1930s in Germany, and over 150 gasifiers have been installed internationally since. Because the Lurgi gasifier is a moving-bed design, the exit gas temperature is lower than for other gasifier designs, and the "cold gas efficiency" (percent of chemical energy in the coal contained in the syngas) is higher.[28] The use of hot gas cleanup (HGCU) eliminates the requirement for syngas cooling typical of many IGCC concepts, therefore preventing the condensation of tars and oils in the raw coal gas and eliminating the associated gas scrubbing equipment, resulting in potentially significant cost savings.[32] The U.S. Department of Energy (DOE) has sponsored a number of system analysis studies to identify potentially promising advanced IGCC process configurations. These include system concepts based upon the dry-ash Lurgi gasifier and HGCU.[32-35] Several IGCC projects under the DOE's Clean Coal Technology (CCT) Program involve components of the simplified Lurgi-based IGCC concept (Black, 1993; Motter and Higginbotham, 1993).[36,37] A simplified IGCC system was evaluated by Frey and Rubin, taking into account uncertainties associated with the performance, emissions, and cost of this commercially unproven concept.[12]

A schematic of the air-blown Lurgi gasifier-based IGCC system with HGCU is shown in Fig. 2. The HGCU system features high temperature fuel gas desulfurization with a zinc ferrite sorbent, and high efficiency cyclones and ceramic filters for particulate removal. The off-gas from the zinc ferrite reactor, which contains sulfur compounds, is sent to a sulfuric acid plant for byproduct recovery. The advantages of such a system, compared to a base case oxygen-blown system with cold gas cleanup (CGCU), are (1) it does not require an expensive and energy consuming oxygen plant, (2) it eliminates fuel gas cooling prior to combustion in the gas turbine, thereby improving the plant thermal efficiency; and (3) it eliminates the need for process condensate wastewater treatment because tars and oils in the fuel gas are not condensed as they would be in a CGCU system. For these reasons, this system concept is "simplified" compared to other alternatives.[32]

In the fixed-bed zinc ferrite process, sulfur is removed from the syngas by reaction with a sorbent consisting of zinc ferrite pellets. Absorption occurs until just before "breakthrough," at which point the sorbent is saturated. The absorber is then taken off-line, and the syngas is diverted to another zinc ferrite reactor vessel containing regenerated sorbent. Sulfided sorbent is regenerated using air as a reactant and steam as a diluent, to prevent the heat released in the exothermic regeneration reactions from sintering the sorbent. The regeneration off-gas containing sulfur dioxide is then processed into sulfuric acid.

3.3 NO_x EMISSIONS FOR IGCC SYSTEMS WITH HOT GAS CLEANUP

Nitrogen oxides are formed in combustion systems through several mechanisms, the most common of which are thermal NO_x and fuel NO_x.[38] Thermal NO_x results from the high temperature fixation of atmospheric nitrogen. Thermal NO_x emissions are expected to be quite low for IGCC systems, due to the low heating value of the fuel gas.[39] Combustor design can also reduce thermal NO_x formation. For example, premixing of fuel and air prior to combustion yields more uniform fuel/air mixtures and minimizes the peak flame temperatures which contribute to thermal NO_x formation.[40]

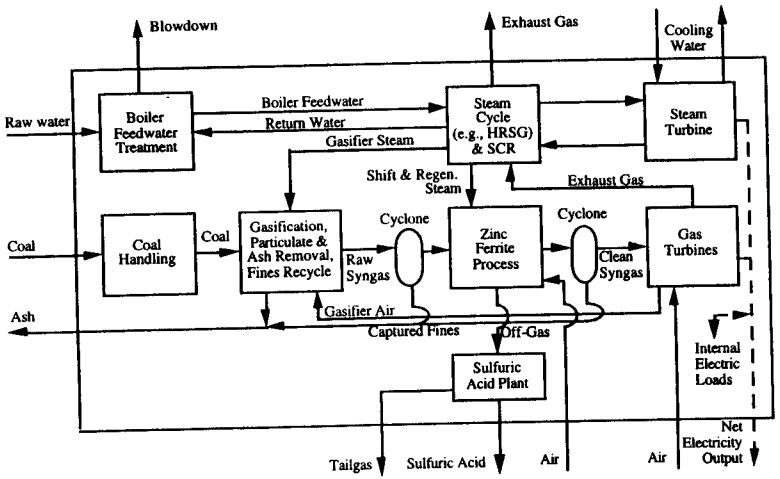

Figure 2. Schematic of Air-Blown Dry-Ash Lurgi Gasifier IGCC System with Hot Gas Cleanup.

However, the fuel NO_x mechanism may be especially important for fixed-bed gasifier IGCC systems with HGCU. Due to their relatively low operating temperatures, Lurgi gasifiers produce a higher amount of ammonia in the coal gas than do other types of gasifiers. The ammonia, which would be captured in a conventional CGCU system during wet scrubbing, passes through the HGCU system unreacted. In a conventional gas turbine combustor, a large fraction of the fuel-bound ammonia would be converted to NO_x. In a previous system study which accounted for uncertainty in estimating the gasifier ammonia yield and the fractional conversion of ammonia to NO_x in the combustor, the 90% confidence interval for the NO_x emission rate was estimated to be between 1.5 and 2.8 lb/10^6 BTU of coal heating value input.[12] The current New Source Performance Standards NSPS for PC power plants are approximately 0.45 lb/10^6 BTU. Thus, the uncontrolled fuel NO_x emissions from this system can be unacceptably high.

To mitigate NO_x emissions, several approaches are possible. Research is underway to develop a new generation of combustor technology to reduce the conversion of fuel-bound nitrogen to NO_x. For example, while conventional combustors may convert 40 to 80% of fuel bound nitrogen to NO_x,[41] conversion rates of 20 to 40% were measured in laboratory testing of an advanced can-annual concept,[42] and preliminary work with staged rich-quench-lean (RQL) has yielded conversions of 40 to 55%.[43] For the RQL design, theoretical expectations are for conversion rates as low as 10%. However, these technologies are not yet ready for the market. Thus, it is necessary to consider the use of postcombustion control as a shorter-term measure.

Postcombustion catalytic control of NO_x has been demonstrated on natural gas-fired gas turbine based systems. Recent commercial experience in Japan and Germany with SCR applied to coal-fired power plants indicates that 80 to 90% NO_x removal may be feasible, although SCR has not yet been applied with U.S. coals.[44] SCR has also been applied to over 80 General Electric natural gas-fired gas turbine systems worldwide.[45] SCR has not yet been applied to coal-fueled gas turbine based systems.

Nitrogen oxides in the flue gas are removed by reduction of NO_x by ammonia to nitrogen and water in the presence of a catalyst. SCR catalysts typically consist of a ceramic honeycomb substrate, a metal "carrier" and active components dispersed by the carrier on the honeycomb surfaces. The actual catalyst formulations which are offered commercially are closely held proprietary information. More detail on SCR is given by Frey[46].

Uncertainties regarding the application of SCR to IGCC systems center on the potential effect of contaminants in the exhaust gas, including catalyst masking, fouling, and poisoning. SCR catalysts oxidize a small fraction of SO_2 to SO_3, which may react with the ammonia slip to form ammonia salts, such as ammonium bisulfate. If formed, this material would likely condense in the cold end of the heat recovery steam generator (HRSG), leading to fouling of heat exchanger surfaces and corrosion problems. Such problems can be minimized by upstream desulfurization and the use of catalyst formulations that decrease sulfur oxidation.

3.4 ADVANCES IN GAS TURBINE TECHNOLOGY

Many IGCC design studies completed during the late 1980s and early 1990s were predicated on heavy duty gas turbine designs featuring a 2,300°F turbine inlet ("firing") temperature and a pressure ratio of 13.5.[12] These assumptions were typical of the GE MS7001F and Westinghouse 501F gas turbines at the time. However, recent operating experience with such gas turbines has led to an uprating of these key performance parameters. For example, the GE MS7001FA is now guaranteed to operate at a pressure ratio of 15.0 and a firing temperature of 2,350°F in natural gas applications.[40] As a result of this uprating, the net power output is increased from 150 MW to 159 MW, and the thermal efficiency is also improved. For coal gasification systems, the lower heating value of the coal gas results in a reduction in the compressed air requirement to deliver a given mass throughput to the turbine inlet nozzle. Therefore, the net power output of the MS7001FA gas turbine when firing coal gas is nominally 192 MW.[47]

3.5 MODELING IGCC SYSTEM PERFORMANCE AND COST USING ASPEN

The performance, emissions, and cost of the IGCC system are modeled using detailed engineering models. A performance model of a simplified Lurgi-based system was developed by DOE using the ASPEN chemical process simulator. This performance model has been significantly modified to more completely and accurately represent process performance and emissions.[48] For example, gas cleanup and gas turbine performance and emissions are more completely characterized in the modified models. A new performance model of selective catalytic reduction (SCR) NO_x control has been added to the IGCC model. Furthermore, new cost models were developed.[49,50]

The cost model was based on approximately 30 design studies of IGCC systems. Direct capital costs are estimated for approximately one dozen major process areas. Typically, several performance and design variables are included in the direct cost models. Indirect and other capital costs are estimated based on approximately 60 cost model parameters. These include process area contingencies, project contingency, indirect construction costs, sales tax, allowance for funds

used during construction, environmental permitting costs, spare parts inventory costs, costs for initial inventories of fuels and chemicals, land cost, and startup costs. Fixed and variable operating costs are estimated based on 40 to 50 parameters. Fixed operating costs include maintenance material and labor for each process area, plant operating labor, and administrative and support labor. Variable operating costs include consumables (e.g., water treatment chemicals, zinc ferrite sorbent), ash disposal, fuel, and byproduct credit. Total levelized costs are calculated using the method of the Electric Power Research Institute (EPRI).[51]

3.6 MODEL INPUT UNCERTAINTIES

There are several types of uncertainty in trying to predict the commercial-scale performance and cost of a new process technology. These include statistical error, systematic error, variability, and lack of an empirical basis for concepts that have not been tested. Uncertainties may apply to different aspects of the process, including performance variables, equipment sizing parameters, process area capital costs, requirements for initial catalysts and chemicals, indirect capital costs, process area maintenance costs, requirements for consumables during plant operation, and the unit costs of consumables, byproducts, wastes, and fuel. Model parameters in any or all of these areas may be uncertain, depending on the state of development of the technology, the level of detail of the performance and cost estimates, future market conditions for new chemicals, catalysts, byproducts, and wastes, and so on.[48]

A unique aspect of the engineering modeling in this study is the use of probabilistic simulation techniques to explicitly represent uncertainties in these advanced technologies, which have not been commercially demonstrated. In many cases, model input assumptions are given probability distributions, rather than single numbers. Examples of the types of distributions that may be employed are shown in Fig. 3. The selection of a distribution depends on the nature of the uncertain variable and the type of information available to estimate its uncertainty.

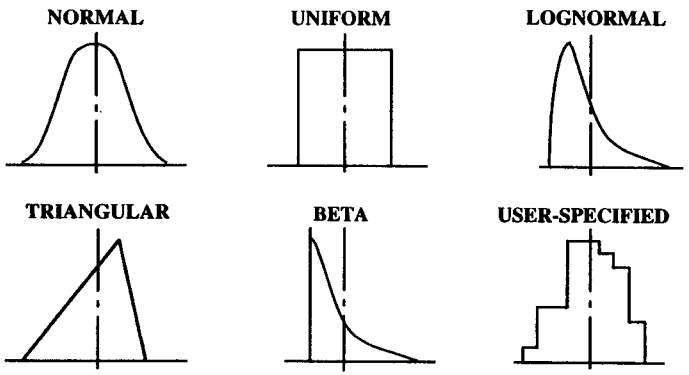

Figure 3. Examples of Probability Distributions Used to Represent Uncertainty in Advanced Process Technologies.

The probability distributions for each input variable are propagated through the models using Latin Hypercube. A new capability has been added to the ASPEN chemical process simulator by Rubin and Diwekar[52] for probabilistic simulation, based on work by Iman and Shortencarier[25].

Key performance and cost parameters of the engineering models for the IGCC system were assigned probability distributions based on data analysis, literature review, or the elicitation of expert judgments. The characterization of performance uncertainties focused on four major process areas: gasification, zinc ferrite desulfurization, gas turbine, and SCR. Uncertainties in additional cost model parameters also were characterized, including direct and indirect capital costs, operating and maintenance costs, financial assumptions, and unit costs of consumables, byproducts, and wastes. The input uncertainty assumptions for the Lurgi-based IGCC system are documented by Frey and Rubin[12]. The input uncertainty assumptions for the SCR system applied to IGCC systems are reported by Frey *et al.*[50] in a case study of a KRW gasifier-based IGCC system. A total of approximately 40 engineering-economic model parameters were initially assigned probability distributions. However, through a process of statistical analysis and iteration, the number of input assumptions treated probabilistically was narrowed to 20. Only those uncertainties which most significantly influenced uncertainty in NO_x emissions, plant thermal efficiency, capital cost, and levelized cost of electricity were retained. These key uncertainty assumptions are given in Table 1. The systems model assumes three heavy-duty gas turbine equipment trains and the use of a bituminous 3.86 weight percent sulfur Illinois No. 6 coal. The purpose of the modeling applications is to evaluate uncertainty in the performance, emissions, and cost of alternative process configurations.

3.7 MODELING RESULTS

The IGCC model was run on a DEC VAXStation 3200 minicomputer using the public version of ASPEN with the new stochastic modeling capability. Model results are reported in Table 2 for an analysis of a system with a 15.0 pressure ratio and 2,350°F firing temperature gas turbine and SCR. The nominal plant size is 710 MW. A few of the results are discussed.

3.7.1 Uncertainties in Process Performance

As shown in Table 2, the plant thermal efficiency is enclosed by a 90% confidence range from 35.7 to 39.6% on a higher heating value coal input basis. In the deterministic analysis, all parameter values were set to a "nominal" assumption, typically representing the mode of the corresponding probability distribution. The results indicate a risk of a 75% chance of lower efficiencies than the deterministic estimate. A contributing factor to this risk is the uncertainty regarding the amount of carbon which is retained in the gasifier bottom ash, which is assigned a positively skewed distribution. Carbon retained in the bottom ash represents a significant efficiency penalty on the IGCC system, because it is not combusted in the gasifier nor converted to fuel gas. The SCR system decreases plant efficiency due to increased gas turbine backpressure, steam consumption required for ammonia vaporization and injection upstream of the SCR catalyst, and electric power consumption required for process area auxiliaries.

3.7.2 Uncertainties in Process Emissions

The results of Table 2 illustrate the low SO_2 emissions typical of IGCC systems. The SO_2 emissions reported here include emissions from both the gas turbine the sulfuric acid plant. The

Table 1. Summary of Deterministic and Uncertainty Assumptions for the IGCC System

DESCRIPTION AND UNITS [a]	DET. VAL.[b]	DISTRIBUTIONS AND THEIR PARAMETERS[c] Type	Min	Max	Mode or Prob.
Gasifier Fines Carryover, wt-% of Coal Feed	5.0	F	0.0	1.0	5%
			1.0	3.5	20%
			3.5	5.0	25%
			5.0	8.0	25%
			8.0	15.0	15%
			15.0	20.0	5%
			20.0	30.0	5%
Fines Capture in Recycle Cyclone, wt-% of Fines Carryover	95	F	50	90	25%
			90	95	25%
			95	97	25%
			97	98	25%
Carbon Retention in the Bottom Ash, wt-%	2.5	T	0.75	10.0	2.5
Gasifier Coal Throughput, lb DAF coal/(h-ft^2)	305	T	152	381	305
Gasifier NH_3 Yield, % of coal-N converted	0.9	T	0.5	1.0	0.9
Gasifier Air/Coal Ratio, lb air/lb DAF coal	3.1	T	2.7	3.4	3.1
Steam/Coal Ratio, lb steam/lb DAF coal					
air/coal = 2.7	0.81	U	0.54	1.08	
air/coal = 3.1	1.55	U	1.24	1.86	
air/coal = 3.4	2.38	U	2.04	2.72	
Zinc Ferrite Sorbent Sulfur Loading, wt-% sulfur	17.0	N	2.16	31.84	17.0
Zinc Ferrite Sorbent Attrition Rate, wt-% sorbent loss per absorption cycle	1.0	F	0.17	0.34	5%
			0.34	0.50	20%
			0.50	1.00	25%
			1.00	1.50	25%
			1.50	5.00	20%
			5.00	25.00	5%
Gas Turbine Pressure Ratio	15.0				
Gas Turbine Firing Temperature, °F	2,350				
Fuel NO_x, % conversion of NH_3 to NO_x	90	T	50	100	90
SCR NO_x Removal Efficiency, %	80				
Gasifier Direct Cost Uncertainty, % of direct capital	20	U	10	30	
Sulfuric Acid Direct Cost Unc., % of direct capital	10	U	0	20	
Gas Turbine Direct Cost Unc., % of direct capital	25	U	0	50	
SCR Unit Catalyst Cost, $/ft^3	840	U	250	840	
Std. Error of HRSG Direct Cost Model, $ Million	0	N	–17.3	17.3	
Maint. Cost Factor, Gasif., % of process area cost	3	T	2	12	3

Table 1. Summary of Deterministic and Uncertainty Assumptions for the IGCC System (continued)

DESCRIPTION AND UNITS [a]	DET. VAL.[b]	DISTRIBUTIONS AND THEIR PARAMETERS[c] Type	Min	Max	Mode or Prob.
Maintenance Cost Factor, Combined Cycle, % of process area total cost	2	T	1.5	6	2
Unit Cost of Zinc Ferrite Sorbent, $/lb	3.00	T	0.75	5.00	3.00
Indirect Construction Cost Factor, %	20	T	15	25	20
Project Contingency Factor, %	17.5	U	10	25	

[a] DAF = dry, ash free; SCR = selective catalytic reduction; HRSG = heat recovery steam generator.
[b] DET. VAL. = deterministic (point-estimate) value.
[c] Four columns are shown to define probability distributions. The first indicates the type of distribution, where F = fractile, T = triangular, N = normal, and U = uniform. The remaining four columns provide the parameters of the distribution. For the fractile, the lower and upper bounds of each range are given, along with the probability of sampling within that range. For the uniform, the lower and upper bounds are given. For the triangular, the lower and upper bounds, and the mode (most likely) value are given. For the normal, the lower and upper bounds of the 95% confidence interval, and the mode, are given.

NSPS for SO_2 from PC power plants is 0.6 lb/10^6 BTU. Thus, this technology can comply with the existing standard.

With the use of SCR designed to achieve 80% removal of NO_x in the gas turbine exhaust, and assuming a conventional combustor that does not attempt to minimize fuel NO_x emissions, it is possible that the IGCC system can be brought into compliance with the current NSPS for coal-fired power plants. The probabilistic estimate of NO_x emissions is shown in Fig. 4 as a cumulative distribution function (cdf). The key input assumptions affecting the emission estimate are the amount of ammonia produced by the gasifier and the fraction of the ammonia converted to NO_x in the gas turbine combustor. These were both assigned negatively skewed distributions. The deterministic estimate, also shown in Fig. 4, is based on the "most likely" or mode values from these distributions. As a result, there is an 85% probability that the NO_x emissions will be lower than the deterministic estimate. There is approximately a 40% probability that the NO_x emissions would exceed the current NSPS. Therefore, additional work may be needed to reduce these emissions.

3.7.3 Uncertainties in Process Economics

Interactions among uncertainties in plant performance and cost parameters lead to uncertainties in key measures of cost used for process evaluation. As shown in Fig. 5, the uncertainty in the total plant capital cost covers a wide range, from about $1,200/kW to over $2,000/kW. The capital cost associated with the SCR system is influenced primarily by uncertainties affecting catalyst requirement and the catalyst unit cost. The mean and median of the plant costs are both approximately $1,450/kW. A deterministic "best guess" analysis of this technology, which did not account for uncertainty, indicated a cost of $1,350/kW. There is a 75% chance that the capital

Table 2. Summary of Results from Deterministic and Probabilistic Simulations of a 710 MW Air-Blown Lurgi Gasifier-Based IGCC System with 2,350°F Gas Turbine, Hot Gas Cleanup, and SCR.

Parameter[b]	Units[c]	Deter. Value[d]	Median $f_{0.50}$	Mean μ	Std Dev σ	Range $f_{0.05}$ to $f_{0.95}$	
Plant Performance							
Thermal Efficiency	%, HHV	38.32	37.4	37.5	1.1	35.7	39.6
Coal Consumption	lb/kWh	0.792	0.812	0.811	0.025	0.767	0.850
Zinc Ferrite Sorbent Charge	10^6 lb	7.37	7.48	8.57	6.08	4.91	13.64
Sulfuric Acid Production	lb/kWh	0.086	0.088	0.088	0.003	0.083	0.092
Process Water Cons.	lb/kWh	1.758	1.741	1.758	0.259	1.302	2.221
Plant Discharges							
SO_2 Emissions	lb/10^6 Btu	0.041	0.040	0.040	0.001	0.038	0.041
NO_x Emissions	lb/10^6 Btu	0.547	0.432	0.437	0.079	0.313	0.569
CO Emissions	lb/kWh	0.003	0.003	0.003	0.001	0.002	0.004
CO_2 Emissions	lb/kWh	1.732	1.729	1.728	0.028	1.680	1.771
Solid Waste	lb/kWh	0.084	0.095	0.098	0.014	0.078	0.125
Plant Costs							
Total Capital Cost	$/kW	1,354	1,434	1,450	145	1,262	1,702
Fixed Operating Costs	$/kW-yr	41.3	53.8	56.1	9.7	42.6	74.8
Variable Oper. Costs	mills/kWh	19.2	19.8	23.0	12.2	17.8	38.4
Coal	mills/kWh	16.3	16.7	16.7	0.5	15.8	17.5
Sulfuric Acid Sales	mills/kWh	(1.5)	(1.6)	(1.6)	0.1	(1.5)	(1.7)
Other	mills/kWh	4.5	4.6	7.9	12.2	3.0	23.2
Cost of Electricity	mills/kWh	51.1	56.5	59.2	14.3	50.8	77.1

[a] The notation in the table heading is defined as follows: $f_n = n^{th}$ fractile ($f_{0.50}$ = median), μ = mean; and σ = standard deviation of the probability distribution. The range enclosed by $f_{0.05}$ to $f_{0.95}$ is the 90% probability range. All costs are January 1989 dollars.
[b] Coal consumption is on an as-received basis. Water consumption is for process requirements including makeup for steam cycle blowdown, gasifier steam, zinc ferrite steam, and SCR. Solid waste includes gasifier bottom ash and nonrecycled fines from fuel gas cyclones.
[c] HHV = higher heating value.
[d] Deterministic value based on a deterministic simulation in which median or modal values of uncertain variables are assumed as "best guess" inputs to the model.

cost would be higher than this estimate, which includes so-called "contingency" allowances intended to account for both performance- and project-related uncertainties. In the probabilistic estimate, contingency factors are replaced with explicit representations of uncertainty in direct costs. Fig. 5 suggests that use of the deterministic cost estimate would expose a decision maker to a substantial chance of a cost overrun.

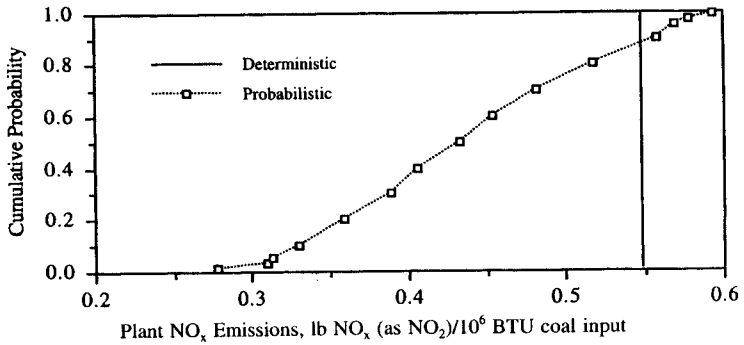

Figure 4. Uncertainty in Total NO_x Emissions from an IGCC System with SCR.

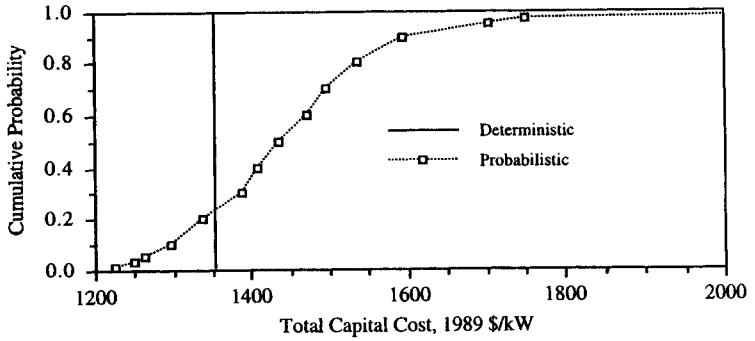

Figure 5. Uncertainty in Total Capital Cost.

The levelized cost of electricity (COE) is the single most comprehensive measure of a plant's economic viability. The uncertainty in the COE is shown in Fig. 6. The risk of poor zinc ferrite sorbent performance is manifested in the long upward tail of the cost uncertainty. The range of uncertainty in the COE varies by a factor of 3 from the lowest to the highest values. In addition, the central values of the probability distribution are higher than the "best guess" estimate. There is approximately a 90% probability that the COE could be higher than the deterministic estimate of 51.1 mills/kWh, due to the interactions of skewed uncertainties and nonlinearities in the engineering model.

3.7.4 Identifying Key Sources of Uncertainty

To illustrate the interactions of different sources of uncertainties, several cdfs are shown in Fig. 6. The "performance only" curve is based on a probabilistic analysis in which all cost-related uncertainties were set to their nominal, point-estimate values. While this distribution has a lower

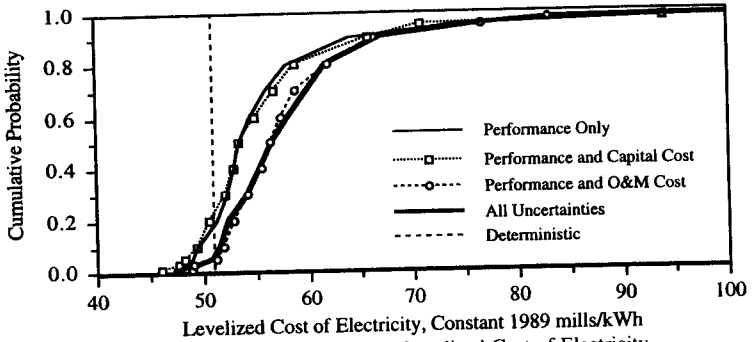

Figure 6. Uncertainty in the Total Levelized Cost of Electricity.

expected value, it nonetheless displays the long tail toward high cost which is a feature of the "all uncertainties" case. Thus, the downside risk of this particular technology is due to performance uncertainties only. Uncertainties in capital cost do not contribute significantly to uncertainty in the levelized cost. However, uncertainties in O&M costs combined with performance uncertainties lead to nearly the same results as when all uncertainties are accounted for. While many capital cost estimates are developed with attention to so-called contingency factors, there is often less attention given to performance or O&M related sources of uncertainty. In this case, this leads to a 90% probability of cost overrun compared to the deterministic estimate.

An alternative approach to identifying key sources of uncertainty is to perform a multivariate regression analysis of the effect of each model input uncertainty on the variance in selected model outputs. Such an analysis is summarized in Table 3. The key uncertainties affecting plant efficiency, total capital cost, and levelized cost of electricity are ranked based on the magnitudes of their respective partial rank correlation coefficients (PRCCs). A mixture of performance and cost parameters significantly impact uncertainty in plant costs. In particular, the uncertainty in the cost of electricity is most sensitive to the zinc ferrite sorbent attrition rate, which is a highly skewed uncertainty. These results provide useful information to technology developers and research planners who wish to increase the payoffs and reduce the downside risks of a new technology. These results indicate that research can be targeted to specific areas to achieve improvements in the technology.

3.7.5 Performance and Cost Impacts of Gas Turbine Characteristics

To evaluate the effect of gas turbine technology, the results from these two simulations were then paired, and the probability distributions for the *differences* between them were estimated. Similarly, two deterministic analysis were performed, and the differences between them were calculated. The effect of the change in gas turbine assumptions from 13.5 pressure ratio and 2,300°F firing temperature to 15.0 pressure ratio and 2,350°F firing temperature is shown in Table 4. The uprated system leads to an average efficiency improvement of 0.5 percentage points. In addition, because of the higher pressure ratio, the mass throughput in the gas turbine is substantially increased,

Table 3. Key Uncertainties for Lurgi-Based IGCC System with 2,350°F Firing Temperature Gas Turbine and SCR Based on Partial Rank Correlation Coefficients (PRCC).

	Selected Output Parameter[a,b]					
Rank	Efficiency		Total Capital Cost		Levelized Cost of Electricity	
Order	Correlated Input Parameters	PRCC	Correlated Input Parameters	PRCC	Correlated Input Parameters	PRCC
1	Carbon Retained in Ash	–0.924	Gasifier Coal Throughput	–0.876	Zinc Ferrite Attrition Rate	0.851
2	Air/Coal Ratio	–0.795	Project Allowance Unc.	0.768	Gasifier Coal Throughput	–0.689
3	Fines Capture in Cyclone	0.630	Gas Turbine Direct Cost	0.703	Zinc Ferrite Sulfur Loading	–0.554
4	Fines Carry Over	–0.408	Zinc Ferrite Sulfur Loading	–0.605	Gasification Maintenance	0.462
5			Indirect Construction Cost	0.572	Carbon Retained in Ash	0.450
6			Std. Error HRSG Model	0.487	Zinc Ferrite Unit Cost	0.426
7			Carbon Retained in Ash	0.451	Gas Turbine Direct Cost	0.405
8			Std. Error HRSG Model	0.416	Carbon Retained in Ash	0.434

[a] Each of the three column lists, in descending order, the parameters most highly correlated with efficiency, total capital cost, or total levelized cost, respectively. The numbers are the partial rank correlation coefficients (PCCs) with respect to the output variable for each uncertain input variable. Abbreviations for uncertain parameters: Std. Error = Standard Error; HRSG = heat recovery steam generator; SCR = selective catalytic reduction.

[b] Only results that are statistically significant are shown, up through the 8th most sensitive input uncertainty.

Table 4. Impact of Gas Turbine Improvements on the Performance, Emissions, and Cost of a Lurgi-Based IGCC System with SCR.[a]

Parameter	Units	Deter. Value[b]	Median $f_{0.50}$	Mean μ	Std Dev σ	Range $f_{0.05}$ to $f_{0.95}$	
Plant Performance							
Increase in Efficiency	%, HHV	0.5	0.5	0.5	0.1	0.4	0.7
Reduction In Costs							
Total Capital Cost	$/kW	129	107	104	24	60	139
Fixed Operating Costs	$/kW-yr	4.8	4.5	4.6	1.4	2.4	7.1
Variable Oper. Costs	mills/kWh	0.3	0.3	0.3	0.2	0.2	0.6
Cost of Electricity	mills/kWh	3.4	3.0	3.0	0.6	1.9	4.0

[a] All values shown are differences between a system with a 2,350°F firing temperature, 15.0 pressure ratio gas turbine and a 2,300°F, 13.5 pressure ratio gas turbine. The notation in the table heading is defined as follows: $f_n = n^{th}$ fractile ($f_{0.50}$ = median), μ = mean; and σ = standard deviation of the probability distribution. The range enclosed by $f_{0.05}$ to $f_{0.95}$ is the 90% probability range. All costs are January 1989 dollars.

[b] Deterministic value based on a deterministic simulation in which median or modal values of uncertain variables are assumed as "best guess" inputs to the model.

which in turn leads to a higher plant output. Using the earlier assumptions, the net plant output is approximately 650 MW, whereas it is increased to 710 MW at the higher pressure ratio. This in turn leads to significant cost reductions. Capital costs are reduced by approximately $100/kW, and levelized costs are reduced by 3.0 mills/kWh. Note that the cost of each gas turbine has not changed, although the costs of all other process areas do change as a result of differences in flowrates through the system. The rating of the gas turbine has improved due to the accumulation of experience with the underlying design, which increased confidence in its performance.

3.8 CASE STUDY CONCLUSIONS

Compared to deterministic analysis, the probabilistic modeling approach requires that more effort be devoted to characterizing the range and likelihood of values assigned to performance and cost parameters in an engineering model. The time required to develop estimates of uncertainty is usually higher than the time that would be required to make a single "best guess" estimate. However, by systematically thinking about uncertainties in specific parameters, an analyst is more likely to uncover potential sources of cost growth or performance shortfalls that are historically overlooked in analyses of new technologies.

The comparison of competing technology options under uncertainty provides insights into their risks and potential payoffs. The simplified Lurgi IGCC with SCR offers the potential of higher thermal efficiency and lower SO_2 and NO_x emissions than conventional coal-fired power plants. However, because of the inability to prevent the formation of fuel NO_x in the gas turbine by eliminating ammonia as a constituent of the fuel gas, there may be a substantial performance and cost penalty associated with the use of SCR systems. The potential for high cost for SCR provides motivation both to improve SCR systems and to seek alternative approaches to NO_x emissions mitigation, such as RQL combustion systems.

4. CASE STUDY 2: INTEGRATED ASSESSMENT OF ACID DEPOSITION

In this section, we present an example of probabilistic analysis for an integrated assessment of acid deposition. This analysis is based upon a publicly available model developed under sponsorship of the U.S. Department of Energy. The model is the "Tracking and Analysis Framework" (TAF). Version 1.7 of TAF was used for the case studies given here. The model was developed by an interdisciplinary and multi-institutional team. The model and additional information regarding the TAF project is currently available on the World Wide Web at http://www.lumina.com/taflist/. The model was developed using Analytica,[‡] which is a probabilistic modeling environment currently available for Macintosh computers. Analytica enables models to be graphically represented as influence diagrams, has built-in capabilities for probabilistic analysis (including Monte Carlo, random Latin Hypercube, and median Latin Hypercube sampling methods), and other features to facilitate model building and execution.

TAF is intended to be a flexible framework for modeling and integrated assessment. The model is illustrated as an influence diagram in Fig. 7. TAF was developed in a modular manner, with different organizations having lead responsibility for specific modules. For example, teams at Argonne National Laboratory had a lead role in the development of the emissions estimation, atmospheric pathways, and visibility effects modules. A team including Carnegie Mellon and Oak Ridge National Laboratory developed the soils and aquatics effects module. A team at Resources for the Future developed the health effects and benefits estimation modules. The software implementation of these modules was guided by Lumina Decision Systems. Several versions of the model were developed and tested to ensure that the inputs and outputs of each module were consistent with other modules in the framework. The software environment is flexible enough to allow users to change the structure of the model or to substitute alternative models within any of the modules.

The purpose of TAF is threefold: (1) support coordination among scientific researchers; (2) support communication with policy makers; and (3) provide guidance for prioritizing research needs. TAF is intended to integrate existing scientific knowledge into a form that can be used by policy makers to compare alternative emissions reduction strategies in terms of their benefits and costs.[53] A variety of alternative emissions projections are built into the model, and there is a provision for users to add their own estimates, as indicated in Fig. 8. The emissions inputs to TAF are broken down by pollutant (SO_2 and NO_x), emission region (states of the U.S., Canadian provinces, and northern Mexico), and five-year time steps from 1990 through 2030. The built-in emissions projections are based upon different assumptions regarding pollution regulations, electricity demand growth rates, and power plant retirement ages. The first of these is a policy assumption. The last two are quantities which are uncertain. Thus, one approach to addressing uncertainty that is used in TAF is to consider different scenarios.

Probabilistic assumptions regarding uncertainties in model inputs are included in several of the modules. The user has the option to select various groupings of quantities for which probabilistic inputs can be used. These sources of uncertainty include stochastic variation in climate parameters that affect either ambient concentrations of pollutants and/or deposition rates, uncertainty in

[‡] Analytica is a registered trademark of Lumina Decision Systems, Inc., Los Altos, California.

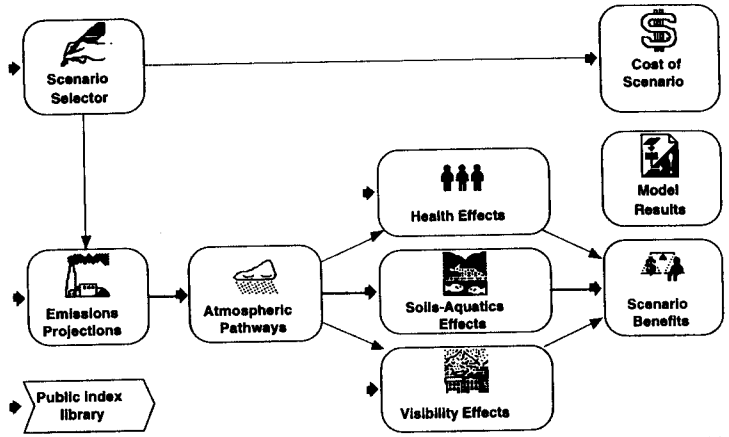

Figure 7. Influence Diagram Illustrating the Implementation in Analytica of the Tracking and Analysis Framework (TAF) for Integrated Assessment of Acid Deposition.

population estimates, and variability in the characteristics of lakes which are one of the receptors of the acid deposition.

In order to run the model, the user must select a baseline and a comparison emissions scenario. In this example, we assume as the baseline a fictional world in which there is no 1990 Clean Air Act Title IV. The 1990 Clean Air Act requires a national emission limit for sulfur oxides and the development of new regulations for nitrogen oxides. This baseline scenario is selected to enable evaluation of the benefits of the comparison scenario with respect to a "do nothing" option. For example, one can estimate the benefits of Title IV by comparison to a scenario in which there is no Title IV.

For comparison purposes, we also consider a case study involving an alternative "aggressive" policy. The aggressive policy assumes a regulation far more ambitious than the current Title IV that may, for example, require flue gas desulfurization to be installed on a much larger number of power plants. We assume for the aggressive policy option that electricity load growth is low and that plant retirements are required after 40 years of operation. Thus, the rate of technology turnover is greater for this case than for the current policy scenario, allowing for more rapid introduction of lower-emitting and higher-efficiency power generation systems (such as the one described in Case Study 1).

The TAF model can be exercised by the user to provide information regarding a variety of benefits at a number of different receptors and times. Examples of benefits include averted morbidity and mortality health effects, averted damages to lakes, and improved visibility in recreational and residential areas. These benefits are presented in various units (e.g., bronchitis cases averted,

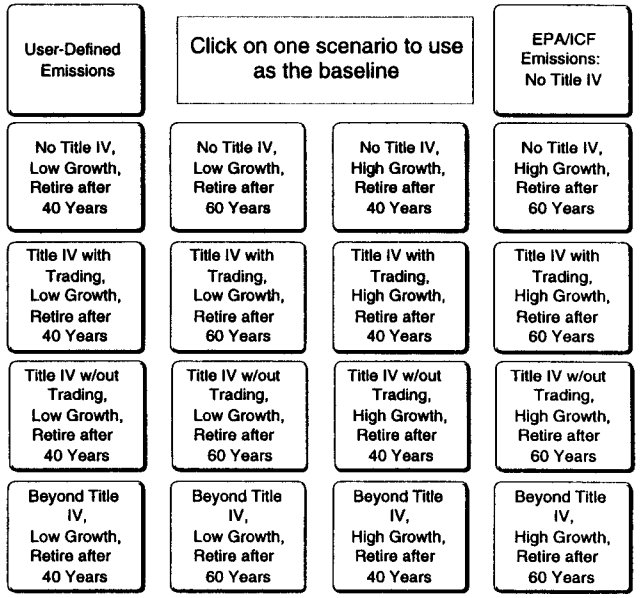

Figure 8. Emissions Scenarios Selector for TAF Model (Version 1.7) as Implemented in Analytica.

deaths averted, etc.). Morbidity, mortality, aquatic, and visibility benefits are also monetized. Thus, there is flexibility regarding the metrics that can be used to report the benefits of a given emission control strategy.

One example of benefits estimation is given in Fig. 9. This figure displays the uncertainty in the prediction of childhood chronic bronchitis cases averted in the year 2010 for all of the receptors included in the model. For the current policy, it appears that anywhere from zero to approximately 300,000 such cases will be averted by the current policy. The more aggressive policy may avert as many as 500,000 cases. These results were obtained using the built-in probabilistic simulation capabilities of Analytica. Clearly, there is a great deal of uncertainty in making estimates of the benefits of air pollution control strategies. Typically, these uncertainties are ignored, and single numbers are used to reflect some type of best guess of unknown pedigree. With a tool such as TAF, it is possible to consider the interactions among uncertainties regarding transport, deposition, exposure, and dose-response to obtain a more representative picture of the current state of knowledge.

The TAF model is an example of the capabilities of the current generation of computers and software. A few years ago it would have been impossible to implement such a large model for

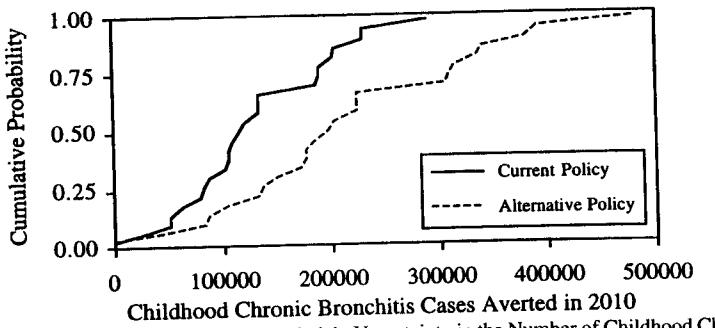

Figure 9. Example Output from the TAF Model: Uncertainty in the Number of Childhood Chronic Bronchitis Cases Averted in the U.S. in the Year 2010.

policy use. The TAF can be executed in a matter of minutes, for relatively small uncertainty analysis sample sizes, and thus can serve as a practical tool to answer a number of "what if" questions regarding the implications of a variety of emission control strategies. Models such as TAF pose a significant challenge to policy makers to better understand what science can and cannot say regarding questions of environmental impacts.

5. CASE STUDY 3: QUANTITATIVE ANALYSIS OF VARIABILITY AND UNCERTAINTY

In this section, several examples are provided regarding a general theme of separating variability and uncertainty. In the previous two case studies, the probabilistic analyses have been explicitly aimed at quantifying uncertainty regarding the ability to make predictions. In Case Study 1, the predictions centered on the performance, emissions, and cost of new technologies. In Case Study 2, the predictions were focused on estimating the national benefits of air pollution control strategies. In this section, we consider situations in which we wish to characterize both variability and uncertainty in model inputs and model outputs. We first begin with a detailed discussion of a simulation-based approach to quantifying uncertainty due to random sampling error. We then present a two-dimensional approach for numerical simulation of both variability and uncertainty.

5.1 QUANTIFYING VARIABILITY AND UNCERTAINTY IN MODEL INPUTS

In this section, we illustrate the distinction between variability and uncertainty using an example data set. The data set has 17 values reflecting variability in the measured PCB concentrations of vine produce at different locations. These data were obtained from Cullen *et al.*[54] While the data contain some measurement error, in this example we focus on characterization of random sampling error assuming that the data are a random representative sample. We employ bootstrap simulation methods, as described by Efron and Tibshirani[55], to characterize the uncertainty regarding the true distribution for variability. Other examples of the use of bootstrap simulation methods for characterization of variability and uncertainty, including an approach for addressing measurement

and random errors, is given by Frey and Rhodes[10]. For the example data set, we first consider the uncertainty in the central moments of the data set. Then we consider the implications of these uncertainties for the selection of parametric distributions to represent the data sets.

5.1.1 Central Moments of Data Sets

The expected value is the first moment of a data set with respect to the origin. Given a random sample of data, the mean is calculated as follows:

$$E(x) = \bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i \tag{1}$$

where E(x) is the expected value (also commonly referred to as the mean, arithmetic mean, average, arithmetic average), x_i is a sample point for the random variable X, and n is the number of data points. Higher-order moments defined with respect to the mean are referred to as "central" moments. In general, the k^{th} central moment for any continuous distribution is

$$\mu_k = E\left[x - \mu_1\right]^k = \int \left(x - \mu_1\right)^k f(x)dx \tag{2}$$

where μ_k is the k^{th} moment about the mean, μ_1. For example, the second central moment, μ_2, is the variance (σ^2), which is a measure of the spread or dispersion of the data. The "unbiased" estimator of the variance (s^2), is given by:

$$s^2 = \frac{1}{n-1}\sum_{i=1}^{n}\left(x_i - \bar{x}\right)^2 \tag{3}$$

Skewness is the asymmetry of a distribution. Skewness is based upon the third central moment of the distribution. The third central moment may be estimated from a dataset using the following relation:

$$m_3 = \frac{\sum_{i=1}^{n}\left(x_i - \bar{x}\right)^3}{n} \tag{4}$$

The skewness, γ_1, is a normalized form of the third central moment with respect to the cube of the standard deviation:

$$\gamma_1 = \frac{\mu_3}{\sigma^3} \tag{5}$$

Skewness may have values that are positive, negative, or zero. For quantities that must be nonnegative, such as concentrations, intake rates, exposure durations, and many other exposure parameters, it is common to have positively skewed distributions that reflect variability. Random measurement errors, on the other hand, may commonly have no skewness. As examples, a normal distribution has a skewness of zero, while a lognormal distribution has a positive skewness. For some purposes, the square of the skewness is used. This quantity is known as β_1:

$$\beta_1 = \left(\frac{\mu_3}{\sigma^3}\right)^2 \tag{6}$$

Kurtosis refers to the peakedness of a distribution. Kurtosis is estimated based upon the fourth central moment of the distribution. The fourth central moment may be estimated from a data set using the following relation:

$$m_4 = \frac{\sum_{i=1}^{n} (x_i - \bar{x})^4}{n} \tag{7}$$

The kurtosis is a nondimensional quantity. It is the fourth moment of the distribution relative to the square of the variance:

$$\gamma_2 = \frac{\mu_4}{(\mu_2)^2} = \frac{\mu_4}{\sigma^4} \tag{8}$$

The kurtosis is also referred to as β_2. A flat distribution, such as the uniform distribution, has a lower kurtosis than a highly peaked distribution, such as the normal or lognormal distributions.

5.1.2 Uncertainty in the Mean, Variance, Skewness, and Kurtosis for Two Example Data Sets

The skewness and kurtosis are useful in helping to select an appropriate parametric distribution to fit a data set. Fig. 10 displays the relationship between the square of the skewness (β_1) and kurtosis (β_2) of many standard parametric probability distributions. The normal distribution always has a skewness of zero and a kurtosis of three and, therefore, is represented as a point on the skewness-kurtosis plane. In the case for which a lognormal distribution has a very small coefficient of variation (σ/μ), the skewness is close to zero and it will appear to be similar to a normal distribution. As the coefficient of variation of the lognormal increases, so will its skewness, and it will deviate from normality.

The mean, selected other central moments, and selected other statistics of the example data set are presented in Table 5. The data are purposefully reported with no more than two digits. In fact, in some cases this may imply far more precision than actually exists regarding estimates for small data sets. As expected, since these must be nonnegative quantities, the data set is positively skewed. The skewness and kurtosis appear to be a close match for a lognormal or gamma distribution. However, an important factor to consider is that with such small sample sizes as for our example data set, there is a substantial amount of uncertainty in the estimates of the skewness and kurtosis.

To more properly characterize the data set, we consider the uncertainty in the mean, standard deviation, skewness, and kurtosis. The uncertainty in a statistic may be represented by a sampling distribution. The sampling distribution for the mean is exactly normal if the true variance (or standard deviation) is known and if the data set is from a normal distribution. The sampling distribution for the mean is related to the student's t-distribution if the data set is from a normal distribution but the true variance is unknown. The sampling distribution for the variance of a data set from a normal distribution is related to the chi-square distribution. When data deviate from these ideal conditions, bootstrap simulation can be used to estimate the sampling distributions. Furthermore, bootstrap simulation can be used for cases in which there may be no theoretical solution.[55]

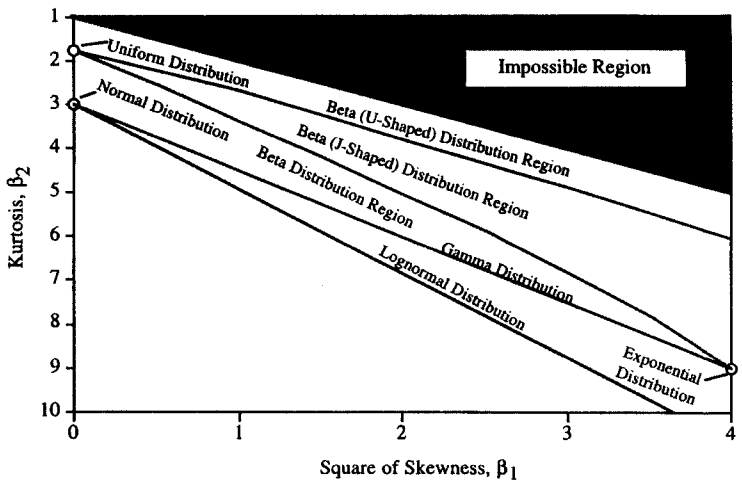

Figure 10. β_1- β_2 Plane Depicting Several Common Parametric Probability Distributions.[13]

Table 5. Examples of Summary Statistics for Data Set of PCB Concentrations in Vine Produce

Description	Value
Number of Data Points	17
Mean, ng/g	0.10
Second Central Moment (Variance), $(ng/g)^2$	0.0022
Third Central Moment, $(ng/g)^3$	1.8×10^{-4}
Skewness	1.7
Fourth Central Moment, $(ng/g)^4$	3.2×10^{-5}
Kurtosis	6.5

Source of Data Set: Cullen *et al.*, 1996

We use bootstrap simulation to estimate the confidence interval for the means of the vine and root produce PCB concentration data sets. Given a data set of sample size *n*, the general approach in bootstrap simulation is to assume a distribution which describes the quantity of interest, to perform *r* replications of the data set by randomly drawing, with replacement, *n* values, and then calculate *r* values of the statistic of interest. For the first step of assuming a distribution for the data set, there are many options. One approach is to use the actual data set itself, and to randomly select, with replacement, the actual values of the data set. This is sometimes referred to as resampling. A second approach is to fit an arbitrary empirically based cumulative distribution function to the data, and to sample from the empirical distribution. For example, one may assume

that the data can be described by a cumulative distribution that is piecewise uniform between each data point. Such a distribution has minimum and maximum values constrained by the minimum and maximum values in the data set. This is referred to here as a fractile distribution. A third approach is to assume a parametric distribution, such as normal or lognormal, to represent the data. Each approach will lead to a different estimate of the confidence interval. We will explore each of these approaches using 1,500 replications.

The results of six different methods for estimating the sampling distributions for the mean of the vine produce data set are shown in Fig. 11. The six approaches provide approximately similar results. If we assume that the underlying data are normally distributed, but that the true variance is unknown, then the student's t-distribution may be used to represent the sampling distribution of the mean. Of the six methods considered, this one yields the widest distribution. Alternatively, if the true variance is assumed to be known, then a normal distribution may be used to represent the sampling distribution of the mean (shown as the "Normal Distribution" case in Fig. 11). This case is nearly the same as that for the student's t-distribution, because with 16 degrees of freedom the student's t-distribution is approximately similar to a normal distribution. The resampling, empirical (fractile) distribution, and normal distribution assumptions for the bootstrap simulation approaches provide similar results to each other and in comparison to the analytically calculated student's t-distribution and normal distribution approaches. If a lognormal distribution is assumed to underlie the data set, then a slightly different sampling distribution for the mean is obtained. This case study demonstrates that it is possible to obtain different sampling distributions for the mean even for a given data set depending on what assumptions the analyst makes regarding the data. In this example, we do not know which one is the "right" answer, if in fact any of these can be considered to be correct. Thus, judgment is involved in selecting and interpreting a method for estimating the confidence interval or sampling distribution.

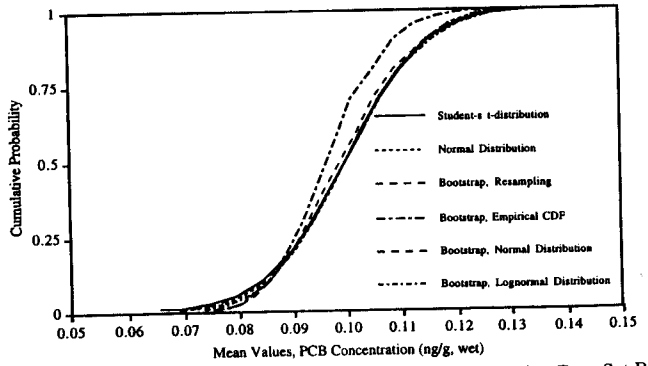

Figure 11. Uncertainty in the Mean of the Vine Produce PCB Concentration Data Set Based upon Alternative Estimation Methods.

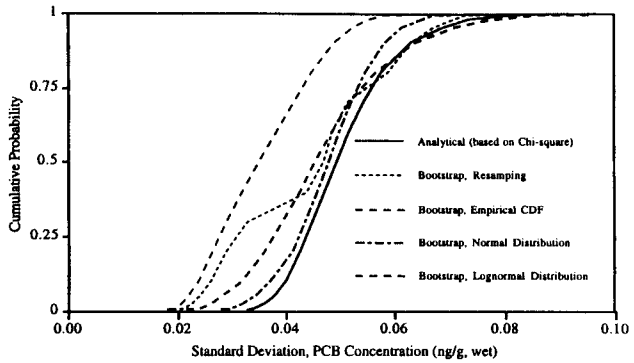

Figure 12. Uncertainty in the Standard Deviation of the Vine Produce PCB Concentration Data Set Based upon Alternative Estimation Methods.

As shown in Fig. 12, the shape of the sampling distribution for the standard deviation depends upon the underlying probability distribution for the population. The cases shown include resampling of the original data set, specification of an empirical distribution for the population using a fractile distribution, and specification of parametric distributions for the data set using normal and lognormal distributions. Furthermore, a sampling distribution for the standard deviation based upon the chi-square distribution for the variance is also shown. The latter would be valid if the data were drawn from a normal distribution. The sampling distribution obtained from resampling of the data appears to have some discontinuities. This is in part because the data set has some repeated values, and because resampling has been done from a data set of finite size. The empirical cdf bootstrap simulation approach gives a confidence interval that tends to be shifted toward lower values than any of the other approaches. This is because there is less chance of simulating the minimum and maximum values for the continuous fractile distribution than there is for the case of resampling. The parametric bootstrap simulations of assumed normal and lognormal populations, and the analytical solution assuming a normal population, give approximately similar results, with slight shifts in the central tendencies. All three of these assume that the population distribution is unbounded for positive values, and the normal case also assumes that the concentrations are unbounded for negative values. Thus, the standard deviations tend to higher for these two cases than for the resampling or empirical cdf cases.

Using the bootstrap simulation methods previously described, estimates of uncertainty regarding the skewness were developed and are displayed in Fig. 13. Of the four cases shown, the resampling, empirical CDF, and lognormal distribution-based approaches provide comparable results. All three of these cases indicate that there is a greater probability that the distribution is positively rather than negatively skewed, and that the skewness may range from approximately -0.5 to 2. In contrast, if the data are assumed to be drawn from a normally distributed population, then the average skewness must be zero and the uncertainty in skewness ranges from approximately -1 to +1 due to random sampling error.

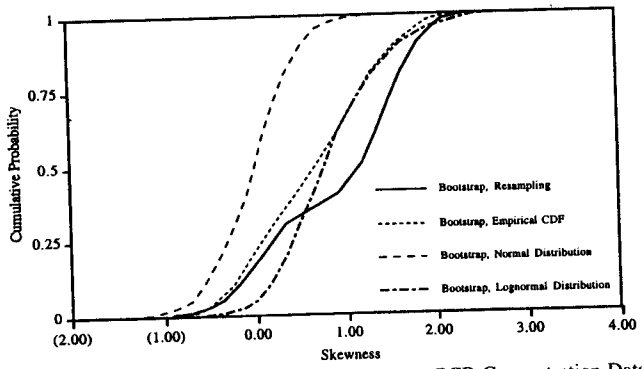

Figure 13. Uncertainty in the Skewness of the Vine Produce PCB Concentration Data Set Based upon Alternative Estimation Methods.

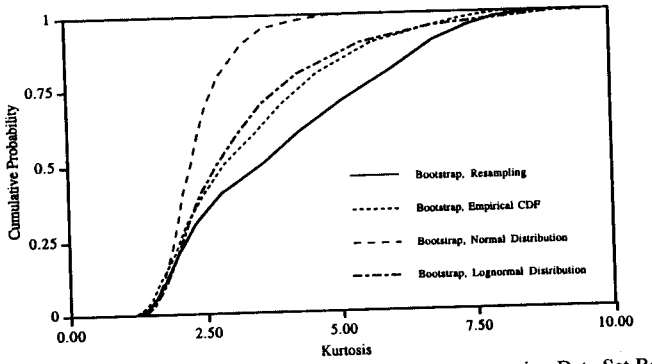

Figure 14. Uncertainty in Kurtosis of the Vine Produce PCB Concentration Data Set Based upon Alternative Estimation Methods.

The results for uncertainty in kurtosis are displayed in Fig. 14. In all four cases, the lower fifth percentile confidence bound for the kurtosis is approximately the same, at a value of approximately 1.5. The 95th percentile upper confidence bound is similar in three of the cases at a value of approximately 8. The primary exception is the case based upon a normal distribution, which is constrained to have smaller values of kurtosis. These results indicate that the uncertainty in kurtosis based upon resampling is more closely related to that of a lognormal than a normal distribution.

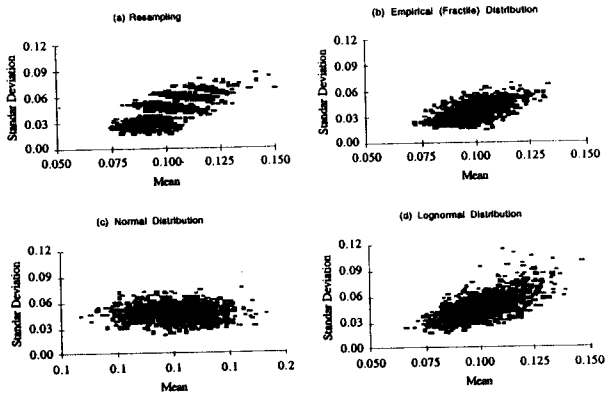

Figure 15. Bivariate Sampling Distributions For Mean and Standard Deviation of an Example Data Set Based upon Four Approaches to Bootstrap Simulation.

5.1.3 Bivariate Sampling Distributions

In the discussion of uncertainty in the mean, standard deviation, skewness, and kurtosis, we have evaluated the implications of different assumptions regarding the distribution that describes the data set for the marginal sampling distributions of each statistic. However, it is also useful to study the multivariate sampling distributions, such as the bivariate distributions for the mean and standard deviation, as shown in Fig. 15, and the bivariate distributions for the skewness and kurtosis, as shown in Fig. 16. The bivariate distributions are displayed as scatter plots of the 1,500 pairs of statistics calculated from the bootstrap simulations. These scatter plots provide an indication of the dependence between the sampling distributions. For example, the mean and standard deviation of a normal distribution are statistically independent. Therefore, the scatter plot of these quantities should be symmetric with respect to both axes, as shown in Fig. 15(c). However, resampling of the data set indicates that there is a positive correlation between the mean and standard deviation. A similar dependence is obtained with either the empirical cdf or the lognormal distribution. Therefore, it would appear that a lognormal distribution might be a more reasonable choice for representing this data set.

The comparison of bivariate sampling distributions for the skewness and kurtosis also indicates that the lognormal distribution may be a better choice than the normal distribution for representing the data set. In addition, the results illustrate that even if the underlying population is positively skewed, it is possible to obtain a data set that appears to be negatively skewed due to random sampling error. For example, in the bootstrap simulation of the lognormal distribution, there were a number of simulated data sets of sample size 17 that had negative skewness. In contrast, because a normal distribution must have a skewness of zero, the average skewness for this case is zero. However, due to sampling error, the skewness can be as high as approximately +1.5 or as low as

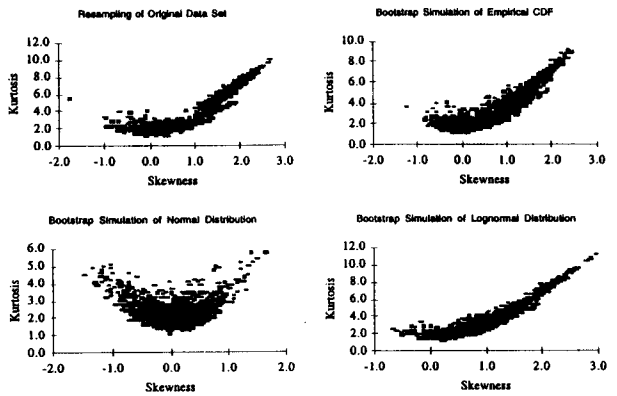

Figure 16. Bivariate Sampling Distributions For Skewness and Kurtosis of an Example Data Set Based upon Four Approaches to Bootstrap Simulation.

approximately -1.5 for a data set of 17 values. Thus, it is possible that a data set that appears to be positively skewed may be a random sample of a population that has zero skewness.

5.1.4 Goodness-of-Fit Tests

A number of goodness-of-fit techniques were applied to evaluate both the normal and lognormal distributions as hypothetical distributions for describing the data set. Probability plots indicated that both distributions provided a reasonable fit to the data, but that the lognormal was a better fit. On the basis of the Kolmogorov-Smirnov test, it is not possible to reject either distribution as inadequate at the 0.05 significance level. The normal distribution can be rejected as inadequate at the 0.05 significance level based upon the Anderson-Darling test. However, it cannot be rejected at the 0.025 significance level. The lognormal distribution can be accepted at these significance levels.

5.2 TWO-DIMENSIONAL SIMULATION OF VARIABILITY AND UNCERTAINTY

As a means for gaining insight into the selection of a parametric distribution to represent the example data set described in the previous section, we simulate the uncertainty in the cumulative distribution function for the fitted distribution due to limited sample size, and compare the probability bounds for the cdf with the original data set. This is done using a two-dimensional approach to probabilistic simulation, as illustrated in Fig. 17.

The two-dimensional simulation approach is based upon that employed by Frey[5]. Given a model, the first step is to disaggregate the model variables into variable and uncertain components. For all variable quantities, frequency distributions must be specified. For all uncertain quantities, probability distributions must be specified. For model inputs that have only variability or uncertainty, only a one-dimensional probabilistic characterization in the variability or uncertainty dimension, respectively, is required for each such input. It is possible to have a number of variable

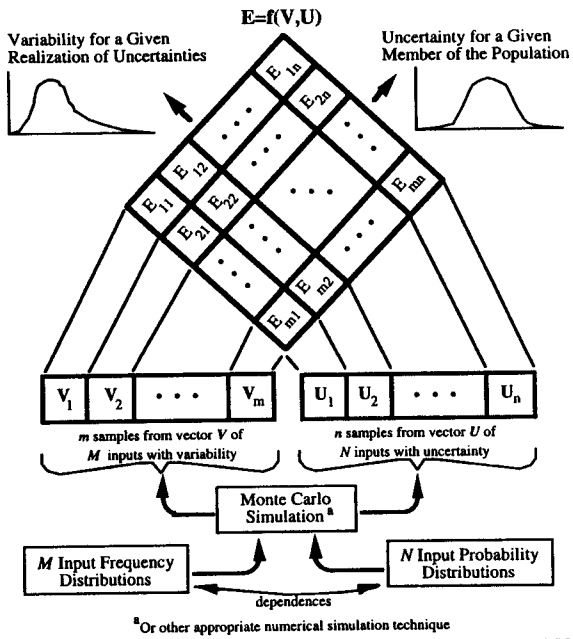

Figure 17. Two-Dimensional Monte Carlo Simulation of Variability and Uncertainty.

input quantities, M, and a potentially different number of uncertain input quantities, N. Thus, it is possible that $M \neq N$. For inputs that are both variable and uncertain, a two-dimensional characterization is required for each input. Possible dependencies between uncertain and variable components of an input are represented by the two-way arc at the bottom of Fig. 17. A sampling technique such as Monte Carlo or Latin Hypercube sampling (LHS) may be employed to generate one or two sets of samples for each model input. The choice of sampling method depends upon the input assumptions. If random sampling error is to be simulated using bootstrap simulation, then Monte Carlo simulation would be employed. In most other cases, LHS would be preferred. In general, different sampling methods can be used in the two dimensions. For each of the M variable quantities, the frequency distributions are simulated with a sample size of m. For each of the N uncertain quantities, the probability distributions are simulated with a sample size of n. In principle, the sample sizes m and n for the variable and uncertain dimensions of the simulation need not be the same. Thus, the sample size for the two-dimensional simulation is m•n.

The model is repetitively evaluated for each combination of samples from the variable and uncertain parameters. This is represented in Fig. 17 by the matrix of values $E_{i,j}$, where i is an index from 1 to m of the sample values for the vector of variable quantities, and j is an index

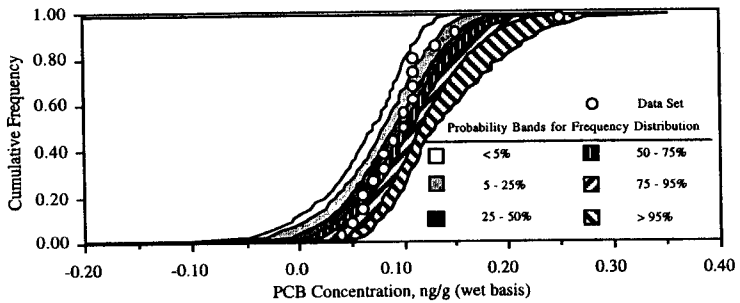

Figure 18. Two-Dimensional Simulation of Uncertainty Regarding the Use of Normal Distributions to Represent the Vine Produce Data Set (n = 17).

from 1 to *n* of the sample values for the vector of uncertain quantities. Any column of the matrix represents the frequency distribution for variability in exposure levels for a given realization of uncertainties for each individual. Any row of the matrix represents the probability distribution for uncertainty in exposure level for a given member of the population.

To evaluate uncertainty regarding the frequency distributions that might be used to describe variability in the PCB concentrations, a subset of the paired values of the mean and variance obtained from the bootstrap simulations previously described were input into the "outer loop" of the two-dimensional simulation. In the "inner loop" of the two-dimensional simulation, a single pair of parameter values was the basis for generating random samples from a fully specified parametric distribution. For illustrative purposes, two different sample sizes were used. For the uncertainty loop, 200 pairs of mean and standard deviation values obtained from the bootstrap simulation were used. The bootstrap simulation was done using Monte Carlo simulation. For each pair of parameter values, 50 samples were drawn from either a normal or a lognormal distribution using median Latin Hypercube sampling. The simulation results were analyzed and are shown in Figures 18 and 19 for normal and lognormal distributions, respectively.

The uncertainty regarding the best fit normal distribution is wide enough to include all of the original data points within a 90% probability range for the cdf, as shown in Fig. 18. Thus, it appears that on the basis of the data a normal distribution is a reasonable fit. The width of the 90% probability band covers a range of approximately 0.10 ng/g, compared to a data set average of 0.10 ng/g. Most of the data points range from 0.05 to 0.15 ng/g. Thus, it appears that the range of uncertainty in the data set is comparable to the observed variability. The main cause for concern with the use of a normal distribution to represent this data set is the significant number of values that are predicted to be below zero, which is physically impossible. For this reason, the normal distribution appears to be inappropriate for this data set.

The lognormal distribution looks like a better fit, as shown in Fig. 19. The range of uncertainty in the cdf is a function of the population percentile. For example, the uncertainty in the upper tails is much wider than for the lower tails. The range of uncertainty is significant with respect

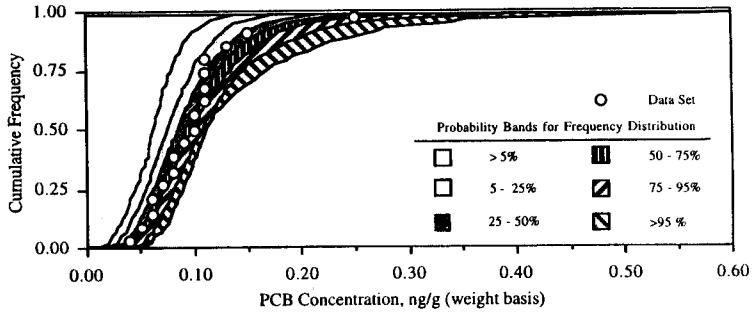

Figure 19. Two-Dimensional Simulation of Uncertainty Regarding the Use of Lognormal Distributions to Represent the Vine Produce Data Set (n = 17).

to the mean and range of the original data set. At the upper percentiles, the upper confidence bound on the uncertainty may be a factor of two greater than the observed data. Thus, it appears that it is important to quantify both uncertainty and variability in this case.

The example results indicate the type of insights that can be obtained from two-dimensional analysis. This approach can be used to quantify the uncertainty associated with any percentile or other statistic of a distribution. In the case of human health risk assessment, for example, we may wish to know how well we can estimate the health risk to the 95th percentile of the exposed population. To specify a point estimate of risk, we would also have to specify a confidence level (e.g., 95% confidence level for the 95th percentile of the exposed population). Comparison of variability and uncertainty can provide insight into whether more research is needed to reduce uncertainty, or whether the assessment should focus on subpopulations that may have unique characteristics compared to the general population. The two-dimensional results can also be used to determine whether exposure or risks are likely to be below levels of concern and, if not, to identify control strategies to protect the most highly exposed or at risk subpopulations.

The example data set presented here was used to explore the use of bootstrap simulation and two-dimensional probabilistic analysis to characterize both variability and uncertainty. Frey and Rhodes (1996) present a more detailed case study of the use of two-dimensional simulation and illustrate a variety of other factors to consider regarding the development of input assumptions, model execution, data analysis, and interpretation of results. Some of the specific factors addressed include the use of mixture distributions, simulation of both measurement and random errors in data sets, effects of correlations, adjustment of data sets for different averaging times, and methods for identifying key sources of variability and uncertainty to prioritize research and data collection.

6. CONCLUSIONS

In this chapter we have described motivations for quantifying variability and uncertainty in the context of energy and environmental systems. General aspects of probabilistic analysis were

presented. Practical aspects of probabilistic analysis were illustrated through a series of three case studies. Many of the shortcomings commonly assigned to probabilistic analysis can in fact be addressed using a variety of methods. This is the case, for example, regarding correlations among model inputs or the identification of key inputs to a model.

The case studies highlight the role that probabilistic analysis can play in conveying limitations in the ability to predict a variety of quantities, such as technology characteristics and the health effects due to acid deposition. In Case Study 1, it was shown that probabilistic analysis can generate insights that affect decisions regarding technology selection and environmental compliance planning. For example, even though on average the performance, emissions, and cost of the example technology may be acceptable, in each case there is a nontrivial risk. Thus, a decision maker may wish to pursue additional research on specific aspects of the technology that contribute most to these risks before adopting the technology for commercial use. In Case Study 2, the use of probabilistic simulation with a large integrated assessment model was demonstrated. The integrated assessment model considers the interactions of uncertainties in several components of the assessment, and clearly conveys the limitations of model predictions through the characterization of uncertainties in model outputs. Case Study 3 illustrates how the distinction between variability and uncertainty may be made in model inputs, and how a two-dimensional simulation method can be used to characterize variability and uncertainty in a model output. The latter is of particular interest in the area of human and ecological exposure to contaminants in the environment, where there is often variability in pollutant concentrations, activity patterns, and characteristics of exposed individuals and uncertainty regarding these due to lack of data, nonrepresentative data, small datasets, and measurement errors.

The most important aspect of probabilistic methods is the insight they provide regarding the strengths and limitations of model inputs and outputs. These methods require more attention to input assumptions than do "best guess" approaches that use point estimates. However, they also produce more scientifically defensible model outputs, information for better decision making, and insight regarding prioritization of additional research and data collection.

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