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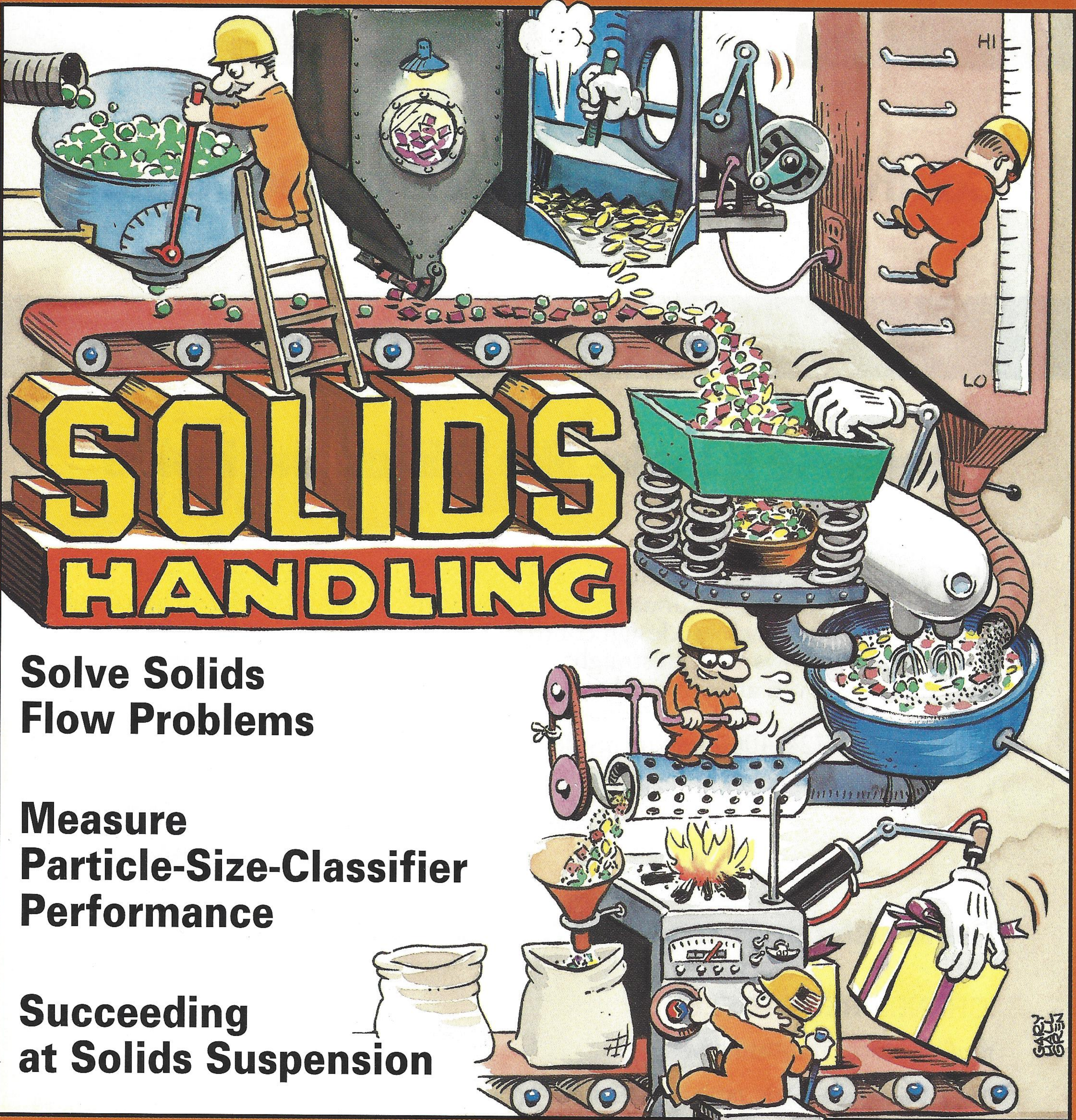

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Evaluate Uncertainties In Advanced Process Technologies

Traditional approaches to technology evaluation inadequately deal with uncertainties. Here is a way to avoid surprises.

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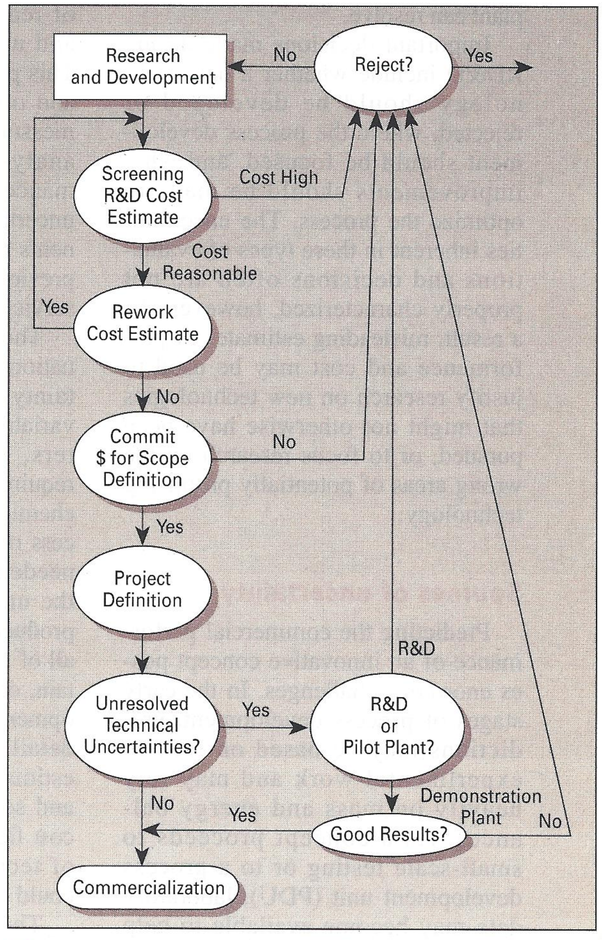
Chemical engineers and technical managers involved in research, development and demonstration (RD&D) of advanced processes can benefit from a systematic approach for characterizing uncertainties in new process technologies. Quantitative characterizations of these uncertainties provide an understanding of the potential performance and cost payoffs of advanced technology, as well as the risks of new technology relative to a baseline commercial system. In addition, detailed uncertainty analysis can allow managers to better focus and prioritize research to reduce technology risks and increase payoffs.

We will describe a methodological approach to uncertainty analysis of advanced chemical process technology performance and cost, and we will discuss the types of insights provided by such analyses. We also will present a detailed case study of an advanced integrated gasification combined cycle (IGCC) power system to illustrate the methodology.



■ *Figure 1. A number of decisions must be made during the RD&D process.*

Decisionmaking during RD&D

Let's first define innovative technology. It is a concept that departs in some fundamental way from existing technology and that holds the promise of a significant improvement in performance or cost. The transformation of an innovative concept into a commercial technology involves many decisions at various stages of development. This is illustrated in Figure 1, based on a discussion in Merrow *et al. (1)*.

Typically, a new concept may be evaluated theoretically and then tested at a small (for instance, bench top) scale. If promising technical results are obtained, a preliminary cost estimate of a commercial-scale design may be made. If the cost appears high, the project may be dropped or research may continue to identify more attractive variants of the technology. If the costs are promising, research is likely to continue to a larger scale of development. Pilot plants of varying size and design may be built and, as confidence in the technology improves, a more definitive cost estimate may be commissioned prior to designing a full-scale plant. At this stage, there still may be significant uncertainties in cost and performance that only a full-scale demonstration plant can resolve.

Important decisions made during RD&D include whether a new technology should be developed or rejected, where the process development should be focused, and what improvements should be made to optimize the process. The uncertainties inherent in these types of evaluations and decisions often are not properly characterized, however. As a result, misleading estimates of performance and cost may be used to justify research on new technologies that might not otherwise have been pursued, or to focus research on the wrong areas of potentially promising technology.

Sources of uncertainty

Predicting the commercial performance of an innovative concept poses enormous challenges. In the early stages of process development, predictions may be based on limited experimental work and may rely heavily on mass and energy balances. As a concept proceeds to small-scale testing or to a process development unit (PDU), laboratory data may become available to help identify more realistic values for key process parameters. Uncertainties in the interpretation of test data, however, may arise from:

1. statistical errors in the data.

2. differences in configuration between the PDU and a commercial-scale plant.

3. potential problems in scale up from the PDU to commercial-size equipment.

The lack of full-scale operating experience to verify predictions of commercial-scale performance of new technology means that many of these uncertainties only can be resolved by building a full-scale demonstration plant at considerable cost.

Uncertainties in key performance parameters of an innovative process give rise to uncertainties in key output characteristics such as plant efficiency, cost, or emissions of pollutants. For example, uncertainties in key system flow rates may lead to uncertainties in the required size of process equipment, the consumption of reagents (for example, sorbent), and auxiliary power requirements. This produces uncertainties in capital and operating costs — the ultimate measures of interest for comparative analysis. Even if process performance were known with certainty, uncertainties regarding many components of cost (such as equipment not previously used in commercial-scale service) would still remain.

Thus, the aspects of a process evaluation that may be subject to uncertainty include process performance variables, equipment sizing parameters, process-area capital costs, requirements for initial catalysts and chemicals, indirect capital costs, process maintenance costs, consumables needed during plant operation, and the unit costs of consumables, byproducts, wastes, and fuel. Any one or all of these parameters 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, and so on. Hence, performance and cost figures developed in early stages of technology development easily could prove incorrect.

The Rand Corporation has studied the problems of estimating the performance and cost of first-of-a-kind innovative process plants *(1)*. Typical of their findings are that:

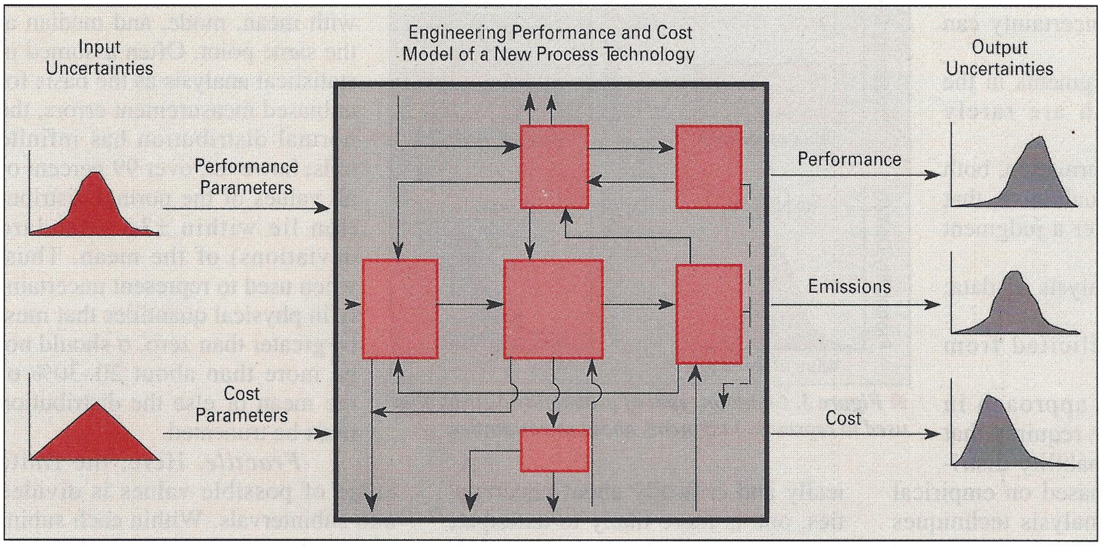
- bias and uncertainty in performance and cost estimates result from low levels of process and project understanding, particularly for new technologies;
- cost-underestimation of new technologies is widespread and systematically related to low levels of project definition and the use of unproven technology; and
- performance over-estimation is also widespread and largely associated with unproven technology in a process concept.

Traditional approaches to handling uncertainty

In developing commercial-scale performance and cost estimates of technologies that are still in early stages of development, the most common approach is for engineers to use a "best guess" point-value for key process and cost parameters for a specified flow sheet. These assumptions may reflect either some degree of optimism or some degree of conservatism. The basis for most assumptions and the scope of thought that went into them typically are not documented, however, in conceptual design studies. Thus, the degree of confidence that should be placed in the performance and cost estimate is often not rigorously considered or reported.

The most common approach to handling uncertainties is either to ignore them or to use simple sensitivity analysis. In sensitivity analysis, the value of a particular parameter is varied across some low to high range, while all other parameters are kept at their nominal values, and the effect on some key output parameter is observed. In practical problems, however, many input variables may be uncertain. The combinatorial explosion of possible sensitivity scenarios (for instance, one variable high, another low, and so on) quickly becomes unmanageable. Because of this, it is often difficult to identify the input variables for which results are most sensitive. Nor is sensitivity analysis able to capture the result of many variables that are uncertain *simultaneously*. Furthermore, sensitivity analysis provides no insight into the *likelihood* of obtaining any particular result across a range of high to low values.

A specific approach to handling uncertainty in capital cost estimates, whether for new or existing technol-



■ *Figure 2. Modeling by representing uncertainties in key input performance and cost parameters as probability distributions allows their effects to be propagated through the model.*

ogy or for preliminary or detailed cost estimating, employs contingency factors. The contingency often is the single largest expense in the cost estimate and yet it is also the least documented or understood. In general, a contingency is used to represent additional costs that are *expected* to occur, but that are not included explicitly in other parts of the cost estimate *(2)*.

In many cases, the approaches used to come up with contingency factors have not been validated by actual data *(3)*. The Rand Corporation conducted a survey of 18 companies in the chemical and petroleum industries to determine the actual methods used to develop contingency factors *(2)*. The study indicates that contingency factors are often badly underestimated and thus may be leading to bad decisions about certain projects. Rand recommends the increased and more formalized use of experience in developing estimates, the use of a delphi technique to get multiple expert inputs, and the inclusion of costs associated with risks and innovation.

Some companies are beginning to use probabilistic modeling approaches to explicitly characterize uncertainties in new process technologies. For example, some studies of advanced-power-generation technologies prepared for the Electric Power Research Institute (EPRI) have included a risk analysis involving probabilistic simulation (for instance, Reference 4). The specification of uncertainties, however, has been only on cost-related parameters. Furthermore, the analysis of uncertainty has been confined just to capital costs, not operating and maintenance costs (which may be a considerable portion of the total cost). Most analyses are insufficiently documented to allow critical evaluation of the modeling results.

A quantitative approach to uncertainty analysis

The potential losses associated with poorly-informed RD&D decisions, and the shortcomings associated with traditional approaches to handling uncertainties, suggest a strong need for quantitative uncertainty analysis in the evaluation of both the performance and cost of advanced process technologies. A number of motivating questions for such an approach include:

1. What is the expected commercial performance and cost based on what is currently known?

2. How reliable are these estimates for mature, commercial plants?

3. What are the key factors driving uncertainty in performance and cost?

4. Which of these factors can be the focus of targeted research to reduce the risks or increase the payoff of the technology?

5. What are the risks and payoffs of the new technology compared to conventional technology?

To answer all of these questions rigorously requires a comprehensive and quantitative approach to uncertainty analysis. Predictions about the performance and cost of innovative technologies should reflect the degree of confidence that engineers have in the input assumptions used to generate the predictions. In this work, the approach taken is to explicitly quantify both the range and likelihood of values for parameters used as inputs to engineering models. Using probabilistic simulation techniques, the effect of *simultaneous* input parameter uncertainties can be propagated through the model to yield an explicit indication of the uncertainty in output values, as illustrated in Figure 2.

Characterizing uncertainties

Estimating uncertainties for new chemical processes involves several steps. These include:

1. reviewing the technical basis for uncertainty in the process.

2. identifying candidate parameters that should be treated as uncertain.

3. determining the source of information regarding uncertainty for each parameter.

4. developing — depending on the availability of information — estimates of uncertainty.

Estimates of uncertainty can be based on:

• published judgments in the literature (which are rarely available);

• published information, both quantitative and qualitative, that can be used to infer a judgment about uncertainty;

• statistical analysis of data; and

• judgments elicited from technical experts.

The classical approach in probability theory requires that estimates for probability distributions must be based on empirical data. Statistical analysis techniques are well known and are not reviewed here. In many practical cases, however, the available data may not be relevant to the problem at hand. For example, test results from a PDU under a given set of conditions may not be directly applicable for estimating the performance of a sixth-of-a-kind commercial scale plant under a different set of operating conditions. Thus, statistical manipulation of data may be an insufficient basis for estimating uncertainty in a real system of interest. Engineering analysis or judgments about the data may be required.

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 or other considerations such as technically-informed judgments *(5)*. The approaches to developing probability distributions for model parameters are similar in many ways to the approach one might take to pick a single "best guess" number for deterministic (point estimate) analysis or to select a range of values to use in a sensitivity analysis. The development of estimates of uncertainty, however, usually requires more detailed thinking about possible outcomes and their relative likelihoods. This is an advantage for the analyst, because by thinking systematically and critically about uncertainties, one is more likely to anticipate otherwise overlooked problems or to identify otherwise overlooked payoffs of a system.

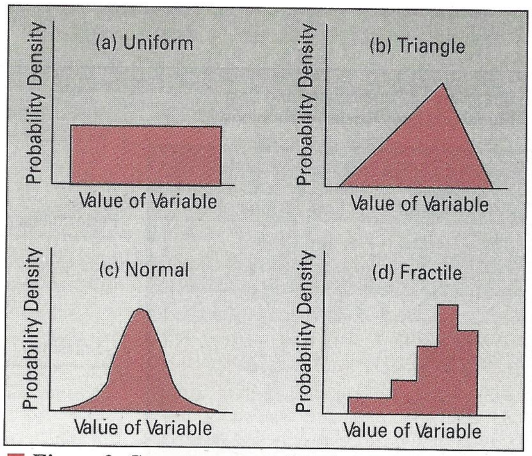


Figure 3. Common types of probability distributions used to represent judgments about uncertainties.

Using probability distributions

In the cases where expert judgments regarding uncertainties are required, an expert may specify a judgment using different types of probability distributions. A few examples are shown schematically in Figure 3. The uses of these are described here briefly:

Uniform. Uniform probability of obtaining a value between upper and lower limits. This distribution is useful when an expert is willing to specify a finite range of possible values, but is unable to decide which values in the range are more likely to occur than others. The use of the uniform distribution is also a signal that the details about uncertainty in the variable are not known. It is useful for screening studies.

Triangle. Similar to uniform except a mode is also specified. Use it when an expert is willing to specify both a finite range of possible values and a "most likely" (mode) value. The triangle distribution may be symmetric or skewed, as in Figure 3(b). Like the uniform, this distribution indicates that additional details about uncertainty are not yet known. The triangle distribution is excellent for screening studies and easy to obtain judgments for.

Normal. A symmetric distribution with mean, mode, and median at the same point. Often assumed in statistical analysis as the basis for unbiased measurement errors, the normal distribution has infinite tails; however, over 99 percent of all values of the normal distribution lie within $\pm 3\sigma$ (standard deviations) of the mean. Thus, when used to represent uncertainty in physical quantities that must be greater than zero, σ should not be more than about 20–30% of the mean or else the distribution must be truncated.

Fractile. Here, the finite range of possible values is divided into subintervals. Within each subinterval, the values are sampled uniformly according to a specified frequency for each subinterval. This distribution looks like a histogram and can be used to represent any arbitrary data or judgment about uncertainties in a parameter when the parameter is continuous. It explicitly shows detail of the judgments about uncertainties.

Probabilistic modeling

In order to analyze uncertainties in innovative process technologies, a probabilistic modeling environment is required. A typical approach is the use of Monte Carlo simulation, as described by Ang and Tang *(6)*, and others. 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, 20–100 or more repetitions are made. The sample size is selected based on the desired precision of the estimate of the output distribution. The result, then, is a set of values for each of the model output variables that can be treated statistically as if it were an experimentally or empirically observed set of data. Appropriate sampling procedures can be adopted to properly account for correlation structures among input variables.

Although the generation of sample values for model input parameters is probabilistic, the execution of the model for a given set of samples is deterministic. The advantage of Monte Carlo methods is that the repetition of deterministic simulations yields important insights into the interactions of many uncertain 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 being restricted to forms that are analytically tractable.

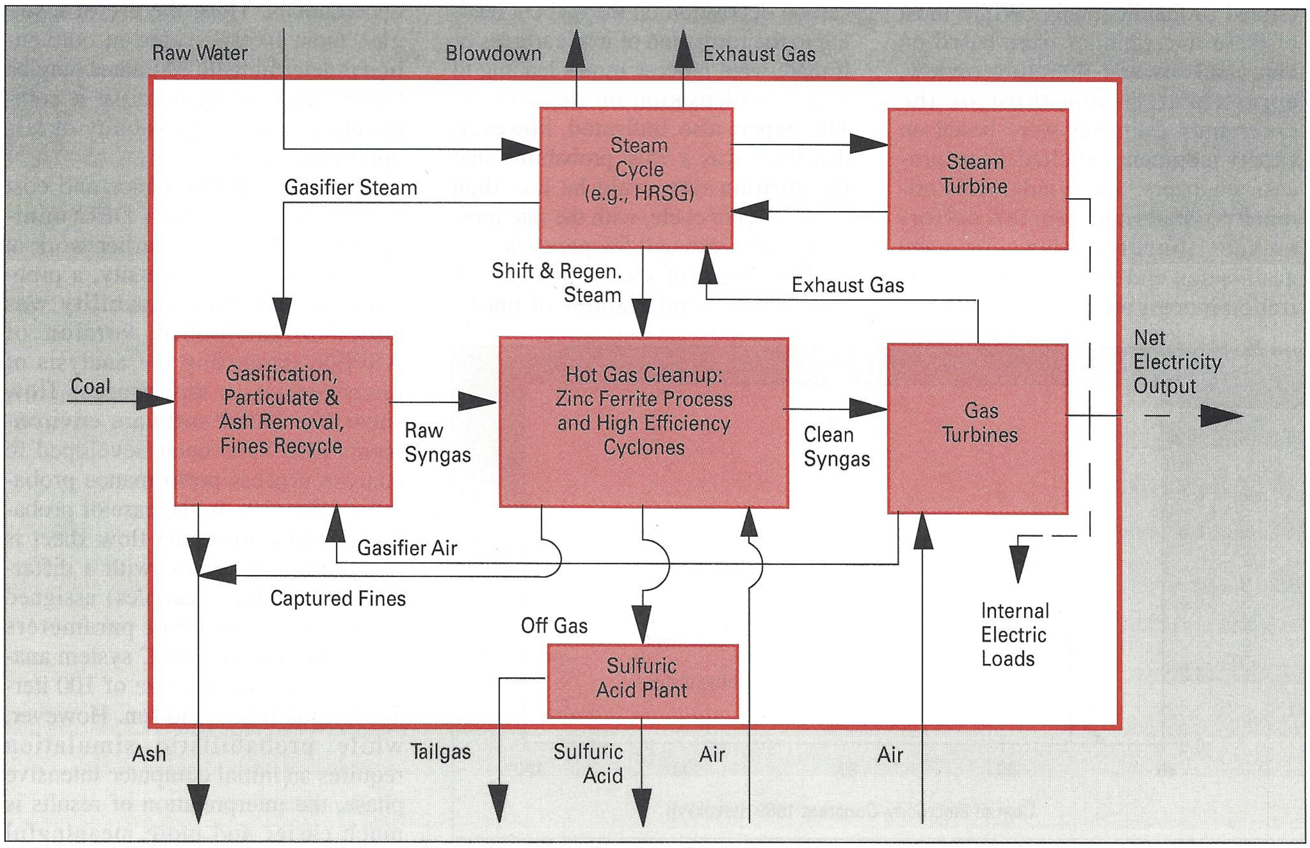
Using Monte Carlo or similar techniques, it is therefore possible to represent uncertainty in a model of a process technology by generating sample values for uncertain variables and running the model repetitively. Instead of obtaining a single number for model outputs, as in deterministic simulation, a set of samples is obtained. These can be represented as cumulative distribution functions and summarized using typical statistics such as mean and variance. Furthermore, the input uncertainties which are the most significant contributors to key results can be identified and ranked using a variety of statistical analysis techniques, such as sample correlation coefficients or multivariate regression.

Thus, probabilistic modeling gives a decisionmaker both explicit measures of uncertainty in key decision variables (for instance, levelized cost or process efficiency) and a listing of key input uncertainties. The former can be used to understand the risks and payoffs of the new technology, while the latter can be used to focus research on reducing the specific input parameter uncertainties that contribute most to the risk of technology failure.

An example

To illustrate the types of insights provided by probabilistic analysis of process technologies in early stages of development, a detailed case study of an advanced integrated gasification combined cycle (IGCC) concept is briefly described. Complete details are available elsewhere *(7)*.

Integrated gasification combined cycle (IGCC) systems are an emerging technology for the clean and more efficient use of coal for electric power generation. Only a few IGCC concepts have been demonstrated at a commercial scale, with many more advanced concepts under evaluation at the laboratory- and small pilot plant scale. One such concept is the air-blown dry-ash Lurgi-gasifier-based system, shown in Figure 4. In this particular design, an advanced dry, high-temperature desulfurization process is used to remove H_2S from the gasified coal prior to combustion of the fuel gas in a gas-turbine combined-cycle system. The desulfurization process uses small pellets of a mixed metal oxide, zinc ferrite, in a fixed-bed reactor that cycles between absorption and regeneration modes.



■ *Figure 4. Schematic diagram of the air-blown Lurgi-gasifier-based IGCC system.*

An engineering performance model of the IGCC concept was developed at the U.S. Department of Energy's Morgantown Energy Technology Center (DOE/METC) using the ASPEN chemical process simulator. The performance model was adopted and modified for this study to better estimate gas-turbine and zinc ferrite desulfurization performance, plant discharge mass-flow rates, and other process parameters required to calculate costs. A key limitation of the DOE performance model was the lack of a directly coupled cost model. Therefore, a cost model was developed based on a review of approximately 30 conceptual design studies of IGCC and similar systems *(8)*. The cost model characterizes direct and total capital cost, fixed operating costs, variable operating costs, and the annualized cost of electricity. The cost model is sensitive to over 100 performance and cost parameters.

For the Lurgi-based IGCC system, 47 parameters in the performance and cost models were characterized probabilistically. While most of these uncertainties were based on data analysis and literature review, approximately one-third of the uncertainty estimates were based on expert judgments elicited from process engineers. These judgments primarily concerned process performance uncertainties in the gasification and zinc ferrite desulfurization process areas.

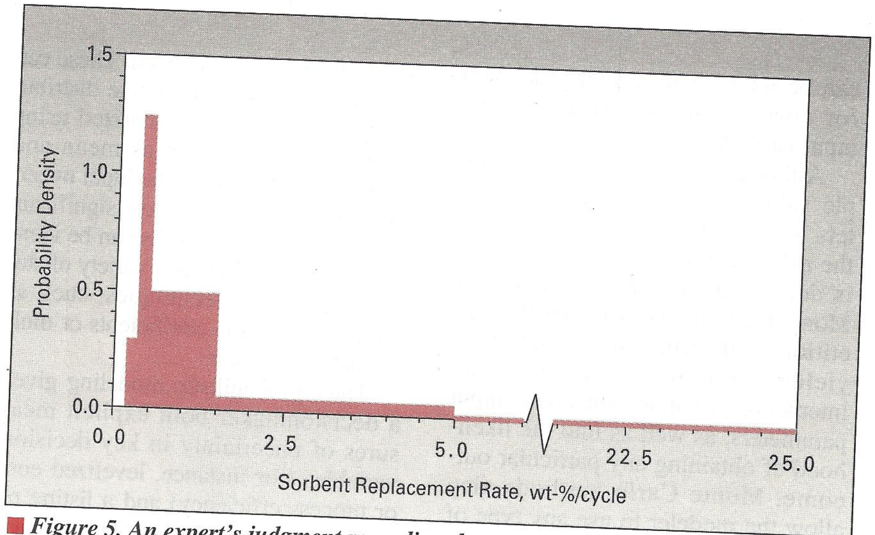


Figure 5. *An expert's judgment regarding the uncertainty in predicting zinc ferrite sorbent attrition rate in a full-scale IGCC desulfurization system.*

An example of one expert judgment — for the uncertainty in the desulfurization-sorbent attrition rate in a future commercial plant — is shown in Figure 5. This is an important parameter since it significantly affects plant cost. This expert indicated that high attrition rates of up to 25% weight loss per absorption/regeneration cycle could occur if there were carbon deposition on the sorbent leading to the formation of iron carbides or if there were process upsets leading to water condensation on the sorbent. The expert also indicated, however, that there was a 75% probability that the attrition rate could be less than 1.5% loss per cycle, with the rate most likely to be around 0.5% per cycle.

The judgment shown in Figure 5 illustrates several features of uncertainty characterization. The expert was able to provide a technical basis for the different values assumed for this particular performance parameter. He also was able to make judgments about the relative likelihood of different outcomes. The resulting probability distribution is skewed, which is often the case when experts are asked to make judgments about uncertainties. Thus, the use of a single "most likely" value in conventional deterministic estimates may be highly misleading because it completely ignores the possibility of less optimistic outcomes.

The IGCC performance and cost models were run on a DEC minicomputer. As part of earlier work at Carnegie Mellon University, a probabilistic modeling capability was added to the public version of ASPEN, permitting the analysis of uncertainties in any process flow sheet *(9)*. Other software environments also have been developed to analyze process performance probabilistically *(10)*. In the case of probabilistic simulation, the flow sheet is executed many times, with a different set of values (samples) assigned to all uncertain input parameters each time. For the IGCC system analyzed here, a sample size of 100 iterations took 6 hours to run. However, while probabilistic simulation requires an initial computer-intensive phase, the interpretation of results is much easier and more meaningful compared to sensitivity analysis.

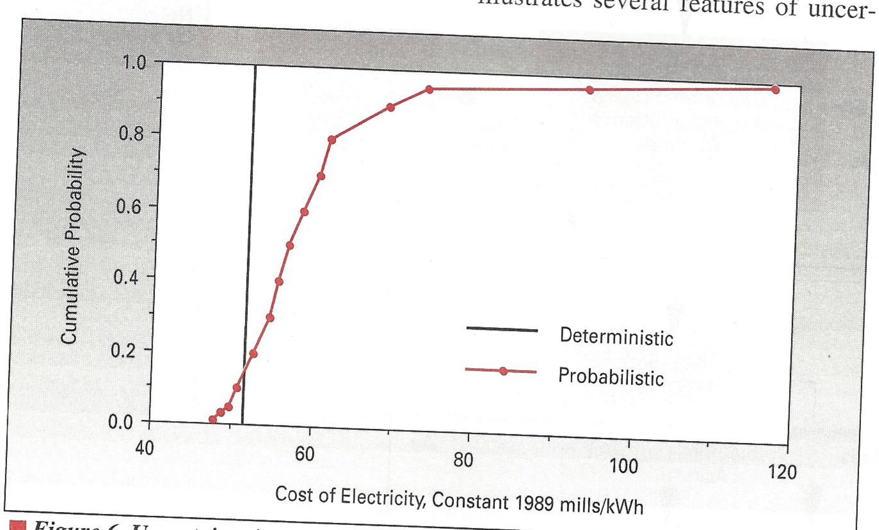


Figure 6. *Uncertainty in the levelized cost of electricity.*

The probabilistic modeling environment can be used to characterize the uncertainty in any desired measure of plant performance, emissions, or cost. For the IGCC system examined here, the levelized cost of electricity is the single most comprehensive measure of interest, because it reflects on (and is sensitive to) all of the factors that determine capital costs, fixed operating costs, and variable operating costs. Because it is expressed on a net electricity-production basis, it is also sensitive to the plant thermal efficiency.

The uncertainty in the net cost of electricity is shown as a cumulative distribution function (cdf) in Figure 6. The ordinate, cumulative probability, shows the probability of being at or below the corresponding abscissa value, cost of electricity. The probabilistic results are based on the propagation of 47 input uncertainties through the model. Also shown is a deterministic estimate based on "best guess" or "most likely" values for all process performance and cost parameters. The range of uncertainty in the total cost varies by a factor of 2.5 from the lowest to the highest values. The central values of the probability distribution are higher than the "best guess" estimate. There is a high probability that the cost of electricity will be higher than the deterministic estimate, due to the interactions of skewed judgments regarding uncertainties and various nonlinearities in the engineering model. In this case, these interactions result in an 85% probability that the cost of electricity will be higher than the "best guess" deterministic estimate, with a 20% probability of exceeding 60 mills/kWh.

Prioritizing research

A benefit of probabilistic analysis is the ability to identify key sources of uncertainty when many parameters are varying simultaneously. These key uncertainties then can be prioritized for further research using statistical techniques such as correlation or regression analysis. The key input uncertainties that affect uncertainty in the total cost of electricity for the IGCC case study are shown in Table 1. These include both performance and cost parameters in the zinc ferrite, gas-turbine, and gasifier process areas. Thus, simultaneous interactions among several process areas are shown to be important here.

Table 1. Key input uncertainties that affect levelized total cost.

1. Zinc ferrite sorbent attrition rate.
2. Zinc ferrite sorbent sulfur loading.
3. Gasifier coal throughput.
4. Gas-turbine direct capital cost.
5. Gasifier maintenance cost.
6. Project-related indirect costs.
7. Zinc ferrite sorbent unit costs.
8. Gasifier direct capital cost.

The interactions among uncertainties also can be illustrated graphically. Figure 7 shows the uncertainty in the cost of electricity resulting from:

1. performance uncertainties only (for instance, mass and energy flows).

2. cost parameter uncertainties only (for example, the unit cost of sorbent or the cost of a specified vessel).

3. the combined interactions simultaneously.

The results in the figure show that the long tail towards high cost is attributable to performance-related uncertainties, while both performance and cost uncertainties have interactive effects on the central values of the distribution. As seen in Table 1, the key performance uncertainties are in the zinc ferrite process area. These uncertainties may be reduced through a targeted research program.

While the results shown here reflect the judgments of one set of technical experts, the analysis easily can be repeated using other experts to identify areas of agreement or disagreement; see *(7)*. For the IGCC system shown here, three sets of expert judgments all led to the same conclusion of a skewed cost distribution, driven primarily by uncertainties in process performance parameters.

Comparing technologies

In the preceding sections, we have focused on applications of uncertainty analysis to an individual technology. The method also is useful for comparing competing technologies. Here, the advanced Lurgi-based system is compared probabilistically to a more conventional IGCC design. In cases where uncertainties are common to both systems (such as interest rates or ash disposal cost), the comparison takes into account the underlying correlation structure.

The probability distribution for the cost savings of the advanced system over the conventional IGCC design is shown in Figure 8. There is roughly a 70% chance that the new technology will be less expensive than the conventional one. Conversely, there is about a 30% chance that the new technology

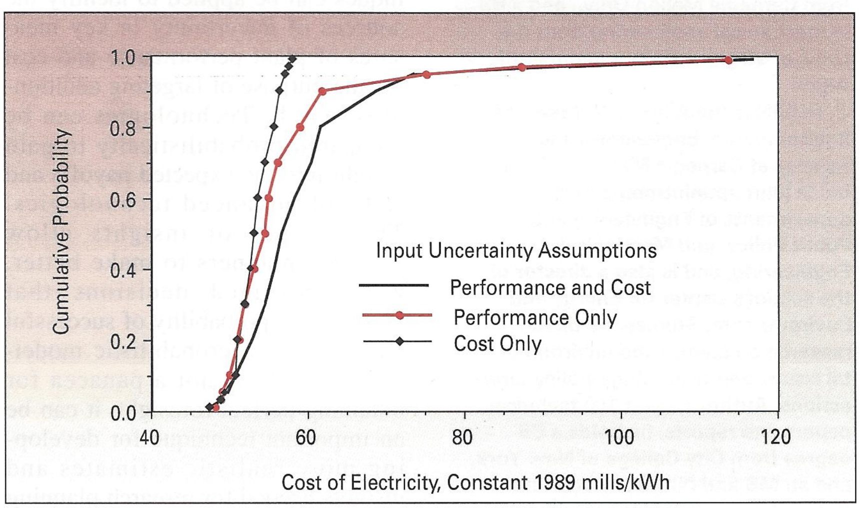


Figure 7. Sources of uncertainty in the levelized cost of electricity.

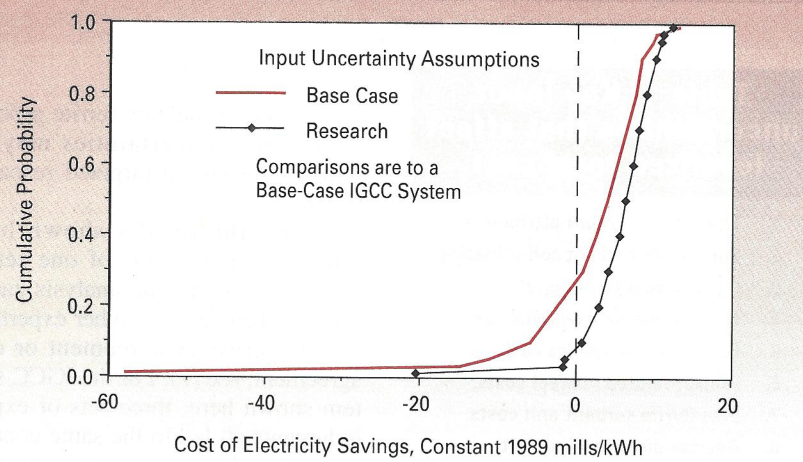


Figure 8. Uncertainty in the cost savings for advanced vs. conventional technology.

could be more expensive, primarily because of potential cost increases in the zinc ferrite process area.

Additional research might change this result, primarily by reducing the risks of the zinc ferrite process. Illustrative research results for three major process areas would increase the probability of cost savings to over 90%. Similar results are obtained even if research simultaneously reduces uncertainties in the conventional technology. Separate analyses also can quantify the expected cost savings with and without research, and the magnitude of the mostly likely downside risks *(7)*.

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Avoiding surprises

Traditional approaches to technology evaluation inadequately account for uncertainties. The result is a history of overoptimistic estimates of performance and cost of new technologies that often lead to significant wastes of time and resources. The probabilistic evaluation method advanced here permits explicit characterization of the uncertainties in performance, emissions, and costs of developing technologies. Many of the "surprises" that account for "performance shortfall" and "cost growth" can be captured by the use of this approach. Quantitative techniques can be applied to identify the sources of uncertainty in key measures of plant performance and cost for the purpose of targeting additional research. Technologies can be compared probabilistically to gain insight into the expected payoffs and risks of advanced technologies. These types of insights allow research planners to make better, more informed decisions that increase the probability of successful RD&D. While probabilistic modeling certainly is not a panacea for obtaining perfect foresight, it can be an important technique for developing more realistic estimates and insights needed for research planning and technology selection. CEP

ACKNOWLEDGMENTS

The work described in this paper was sponsored by the U.S. DOE through the Morgantown Energy Technology Center under contract DE-AC21-88MC24248. The authors are solely responsible for the content and assumptions of this article.

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