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MODELING UNCERTAINTIES IN ADVANCED TECHNOLOGIES: APPLICATION TO A COAL GASIFICATION SYSTEM WITH HOT-GAS CLEANUP

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Abstract—Uncertainties in the performance, emissions, and cost of advanced process technologies in early stages of development pose a challenge to process evaluation. Failure to account properly for uncertainties may result in misleading estimates that are then used for making decisions about technology selection and research planning. A new stochastic modeling capability has been developed for the ASPEN chemical process simulator that allows uncertainties in any process technology to be represented using probability distributions. This capability is briefly described. A detailed case study of an advanced integrated coal gasification combined cycle (IGCC) system is presented to illustrate the application of this capability. The case study involves identification and characterization of uncertainties in model inputs, propagation of uncertainties through the model, and interpretation of model results. The value of stochastic modeling is in the ability to evaluate the *simultaneous* effect of multiple uncertainties in a process technology and to develop more realistic estimates of process performance and cost than would otherwise be obtained from deterministic (point-estimate) analysis.

INTRODUCTION

Advanced process concepts tested only at bench- or pilot-scales lack the large-scale commercial operating experience required to verify predictions of performance and cost.[1] In spite of this, performance and costs of new technologies often are estimated as deterministic point-values, without regard to their uncertainty. Thus, estimates that may be accurate only within a factor of 2 or 3 are often misrepresented as single point-values with several decimal places. Deterministic estimates of both performance and cost for advanced technologies are also known to have a systematic bias toward optimism.[2] An important challenge for process modeling, therefore, is to characterize explicitly and simulate the uncertainties that lead to risks of cost growth and performance shortfall in new process concepts.

Process modeling of advanced technologies must be able to address questions regarding the following: the uncertainty in key measures of plant performance and cost used as a basis for decision making; identification of robust design solutions under uncertainty; identification of key problem areas that should be the focus of further research to reduce the risk of technology failure; comparison of competing technologies on a consistent basis to determine the risks associated with advanced technology; and evaluation of the effects that additional research might have on comparisons with conventional technology.

A probabilistic process modeling approach is described in this paper which allows the explicit and quantitative representation of uncertainties inherent in advanced technologies. As part of this work, a probabilistic modeling capability has been added to the publicly available version of ASPEN, a chemical process simulator. Both methodological and practical issues related to probabilistic process modeling are illustrated using a detailed case study of a coal-based advanced integrated gasification combined cycle (IGCC) concept. The case study illustrates the

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application of probabilistic process simulation to estimation of uncertainty in plant performance and cost, prioritization of key uncertainties for further research, and design analysis under uncertainty. The data requirements for probabilistic analysis are discussed. This method is shown to be a versatile tool for technology evaluation, cost estimating, process design, risk assessment, research planning, and technology selection.

NEED FOR UNCERTAINTY ANALYSIS

Nearly all analyses of process technologies that are in early phases of research involve uncertainties. According to the Rand Corporation, "accurate assessment of the costs of advanced technologies has always been one of the most difficult and uncertain tasks facing an R&D planner."[3] Predictions of the future commercial-scale performance of a new technology are often based on limited experimental data from small-scale testing. Predictions of future cost are typically expressed as deterministic point-value estimates based on assumed values of key performance and design variables, without regard to their uncertainty. Such performance and cost estimates of a new technology, however, are inherently uncertain because of the lack of large-scale experience to verify expectations. Misleading estimates of the performance and cost of new processes can have deleterious implications for research planning and the allocation of resources to the development of alternative technologies.

Thus, the ability to analyse uncertainties is especially important in the context of ongoing research and development, where technical and economic parameters for individual processes and system designs are not well-established. Uncertainties also are important in comparing advanced system designs with baseline systems reflecting currently commercial technology. To analyse uncertainty, the capability to perform sensitivity analysis through a series of multiple runs is usually available. Typically, however, only one or two parameters at a time are varied in a simulation framework which may contain a large number of independent variables. Thus, important interactions or cases may be overlooked. The combinatorial explosion of possible sensitivity scenarios (e.g., one variable "high", another "low", and so on) may make results cumbersome or difficult to interpret and/or display. Furthermore, sensitivity analysis provides no information as to the *likelihood* of different outcomes. In short, the process analysis of real systems requires both stochastic and deterministic modeling capabilities.

Though uncertainty analysis techniques are gaining attention in the literature, none of the well-known process simulators have the capability to handle uncertainties systematically. Conventional chemical process simulation models, such as FLOWTRAN, PROCESS, CHEMSHARE, and ASPEN, typically employ a Fortran code which produces deterministic (point estimate) results for a particular set of input assumptions.[4] Such an approach can be overly simplistic, however, because it ignores uncertainties often known to exist in process performance or design, particularly for advanced technologies.

STOCHASTIC MODELING OF CHEMICAL PROCESSES USING ASPEN

A new stochastic modeling capability for uncertainty analysis has been added to the public version of the ASPEN simulator developed for the U.S. Department of Energy.[4,5] To implement the stochastic modeling capability, ASPEN's modular nature (consisting of unit operation modules or blocks) has been utilized. The stochastic simulation module is based on public domain programs by Iman and others.[6,7] A new unit operation block, called STOCHA, has been added to the ASPEN unit operation library. The structure of this block and its use are briefly described. Details are provided elsewhere.[8]

The unit operation block, STOCHA, characterizes the uncertainty in model input parameters in terms of probability distributions, and analyses their effect on selected output

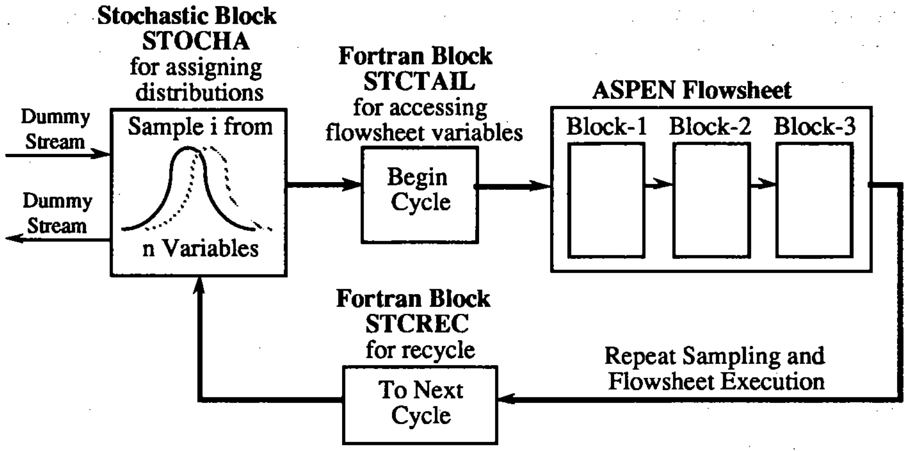

Fig. 1. Basic operation of the stochastic simulation method.

variables. To link STOCHA to the ASPEN flowsheet, two Fortran blocks are needed. The stochastic modeling approach involves the following steps: (i) specification of uncertainties in key input parameters in terms of probability distributions; (ii) specification of the correlation structure of any interdependent parameters; (iii) sampling of the distributions in an iterative fashion, using random Monte Carlo simulation or Latin Hypercube sampling (see Ang and Tang,[9] Iman and Shortencarier,[6] or Morgan and Henrion[10]); (iv) propagation of the effects of uncertainties through the process flowsheet; and (v) application of graphical and statistical techniques to analyse the results.

Figure 1 shows the use of the stochastic block for uncertainty analysis of a flowsheet. The cycle for stochastic simulation consists of: (a) the stochastic block, STOCHA, for generating i samples from the probability distributions for n uncertain flowsheet variables selected by the user; (b) the Fortran block, STCTAIL, for accessing the uncertain flowsheet variables at the beginning of a repetition and assigning to them the sample values from their associated probability distributions; and (c) the Fortran block, STCREC, for data output collection and recycling to the next repetition.

A variety of types of probability distributions for characterizing uncertainties are available in the Fortran program developed by Iman and Shortencarier.[6] Examples of some of these distributions are shown in Fig. 2. Details regarding the basis for using various types of probability distributions are given by Morgan and Henrion,[10] Frey[1] and Frey and Rubin.[11]

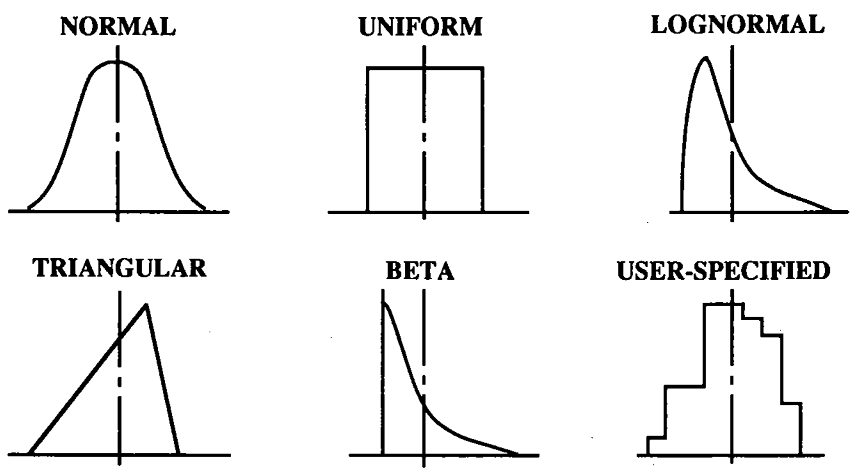

Fig. 2. Examples of probability distribution functions available for stochastic simulation in ASPEN.

Once the input samples have passed through the flowsheet and all the sample runs are completed, the stochastic block can be used to quantify the sensitivity of an output to each input parameter. Four techniques are available for this purpose, all based on multivariate linear regression analysis. These include partial correlation coefficients, standardized regression coefficients, partial rank correlation coefficients, and standardized rank regression coefficients. These are discussed in detail by Iman et al,[7] and summarized by Diwekar and Rubin[4] and Frey.[1]

A DETAILED CASE STUDY

The stochastic modeling capability for the ASPEN simulator is applied here to a detailed case study of an advanced IGCC concept. The case study illustrates the use of stochastic modeling for characterizing uncertainty in key measures of process viability, identifying key uncertainties that can be prioritized for further research, and comparison of alternative process designs.

IGCC technology

IGCC systems are emerging technologies for the cleaner and more efficient use of coal for power generation. These systems feature: conversion of coal to a fuel gas by reaction with steam and oxygen in a pressurized reducing atmosphere; cleanup of the fuel gas to remove particulates, sulfur compounds, and other contaminants; and combustion of the fuel gas in a gas turbine combined-cycle system. IGCC systems are capable of higher thermal efficiency and lower gaseous, liquid, and solid discharges than conventional pulverized coal-fired power plants.[12] However, few IGCC systems have been commercially demonstrated. Those that have been demonstrated feature entrained-flow gasifiers using "cold" (100°F) wet fuel gas-cleanup technology.[13,14] For many other IGCC concepts that are in early stages of development, there are uncertainties regarding process performance, emissions, and cost that may not be resolved until a commercial-scale demonstration plant is built. Uncertainties are particularly important for many advanced concepts featuring high temperature "hot" (e.g., 1000°F) dry fuel gas-cleanup technology. Hot-gas cleanup offers the potentially key advantages of higher plant thermal efficiencies and lower costs due to the elimination of fuel gas cooling and associated heat exchangers.[15]

A promising hot-gas cleanup configuration is an air-blown Kellogg–Rust–Westinghouse (KRW) IGCC system.[16] A schematic of this technology is shown in Fig. 3. The hot-gas cleanup system features in-bed desulfurization in the fluidized bed gasifier with limestone or dolomite, subsequent sulfur removal from the fuel gas 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 recycled to the gasifier. The advantages of such a system, compared to a base case oxygen-blown system with cold-gas cleanup, are: (i) it does not require an expensive and energy-consuming oxygen plant; (ii) it eliminates the capital costs associated with sulfur recovery (all sulfur is disposed with the spent limestone or dolomite); and (iii) it reduces the amount of fuel gas cooling required prior to combustion in the gas turbine, thereby improving the plant thermal efficiency.

Testing of an air-blown KRW-based system with hot-gas cleanup at the process development unit (PDU) level has been conducted.[17] M. W. Kellogg has presented some results of a conceptual performance and cost analysis of such a system, although no detail was provided on costs.[18] M. W. Kellogg and Bechtel, under a cooperative agreement with DOE as part of the clean coal technology program, began design of a 63.5 MW demonstration plant of a KRW gasifier IGCC system with hot-gas cleanup using the fixed-bed zinc ferrite process, although actual construction and testing of that project did not occur.[17,19] Conceptual performance and

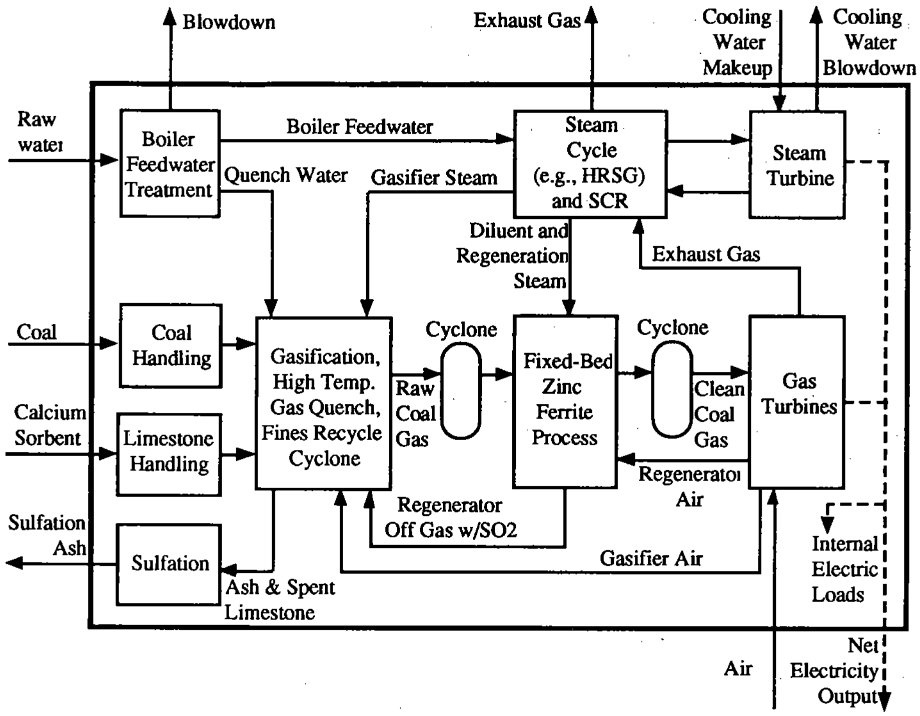

Fig. 3. Simplified schematic of the air-blown KRW gasifier IGCC system with hot gas cleanup.

cost estimates of similar systems have also been prepared by Southern Company Services and Fluor Daniel.[19,20] A demonstration project for a 86 MW subbituminous coal-fired plant with hot-gas cleanup is planned by Sierra Pacific Power Company.[21]

Modeling performance and cost

The performance, emissions, and cost of the IGCC system are modeled using detailed engineering models. A performance model was originally developed by DOE's Morgantown Energy Technology Center (DOE/METC) using the ASPEN chemical process simulator. The performance model has been significantly modified to represent more completely and accurately process performance and emissions.[1] A new performance model of selective catalytic reduction (SCR) NO_x control has been added to the IGCC model.[22] Furthermore, a new cost model was developed.[1,23,24]

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 40–50 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 financial assumptions and methodology of EPRI.[25]

INPUT UNCERTAINTY ASSUMPTIONS

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, and future market conditions for new chemicals, catalysts, byproducts, wastes, and other process components.[1,11]

It may not always be possible to develop estimates of uncertainty based on classical statistical analysis, nor would such an approach be appropriate in many cases. Particularly for new process technologies, data may be lacking regarding some types of uncertainty. For example, the effect of scale-up on process performance may not be fully understood. Thus, analysis of bench-scale test data alone may be an insufficient basis for estimating the total uncertainty in a variable. When data are lacking, estimates of uncertainty must rely on the informed judgments of technical experts. Judgments regarding uncertainties can be encoded as probability distributions, using techniques discussed elsewhere.[10]

Uncertainties in specific performance and cost parameters were explicitly characterized using probability distributions. Identification of parameters that should be treated probabilistically, and the estimates of uncertainties for these parameters, were based on literature review, data analysis, and elicitation of expert judgments from METC process engineers involved in technology development. This approach has also been applied by Frey and Rubin for evaluating a fixed-bed gasifier-based IGCC system.[26]

The characterization of performance uncertainties focused on five major process areas: gasification, sulfation, 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. These assumptions are given in Table 1. Details of the assumptions are provided elsewhere.[1,22]

Technical experts at METC provided judgments regarding uncertainties in the zinc ferrite desulfurization process area. Because the experience of the METC experts was strongly performance-oriented, and less cost-oriented, the focus of the uncertainty elicitations was on performance. A briefing packet was developed and distributed to each METC expert. The packet consisted of three parts: (i) a nine-page introduction to uncertainty analysis; (ii) a 10-page technical background paper on the zinc ferrite process area, with focus on specific aspects that may be uncertain; and (iii) a written questionnaire asking for uncertainty judgments for specific model parameters. After the questionnaires were returned, a follow-up phone interview was used to clarify some responses. The responses were then encoded into the model as probability distributions.[1]

The IGCC models were run on a DEC VAXStation 3200 mini-computer using the public version of ASPEN with the new stochastic modeling capability.[4] A deterministic analysis may take approximately 20–30 min to run, including input translation and other steps. For a probabilistic simulation, the flowsheet is executed many times, with a different set of values (samples) assigned to uncertain input parameters each time. Thus, a probabilistic analysis with a sample size of 100 may take 12 h to run. However, while stochastic simulation requires an initial computer-intensive phase, the interpretation of results is much easier and more meaningful compared to sensitivity analysis.

MODELING RESULTS

The engineering models were exercised in the probabilistic modeling environment to characterize uncertainties in key measures of plant performance, emissions, and cost, based on

Table 1. Summary of the base case deterministic and uncertainty assumptions for the advanced IGCC system.

DESCRIPTION AND UNITS	DET.† VALUE	DISTRIBUTIONS AND THEIR PARAMETERS‡				
GASIFIER						
Gasifier Pres., psia	465					
Gasifier Temp., °F	1,900	T	1,900	to	1,950	(1900)
Overall Carbon Conversion, wt-%	95	T	90	to	97	(95)
O_2/C Molar Ratio	0.46	T	0.45	to	0.47	(0.46)
H_2O/O_2 Molar Ratio	0.45					
Sulfur Capture, mol-% inlet sulfur	90	T	85	to	95	(90)
Ca/S Molar Ratio	2.6	T	2	to	2.8	(2.6)
Ammonia Yield, fraction of coal N	0.10	T	0.005	to	0.10	(0.10)
SULFATION						
SO_2 Emissions, lb/MMBtu	0.01	T	0.01	to	0.05	(0.01)
NO_x Emissions, lb/MMBtu	0.15	T	0.10	to	0.20	(0.20)
Conversion of CaS to $CaSO_4$, %	60	U	30	to	90	
Carbon Conv., %	95	T	90	to	98	(95)
ZINC FERRITE DESULFURIZATION						
Resid. Sulfate after oxid. regen, mol-% of captured S	7.5	T	3	to	11	(7.5)
Resid. Sulfide after red. regen., mol-% of captured S	85					
Sorbent Sulfur Loading, wt-% S	17	N	2.16	to	31.84	(17)
Sorbent Attrition, wt-%/cycle	1.0	F	5%: 0.17	to	0.34	
			20%: 0.34	to	0.5	
			25%: 0.5	to	1	
			25%: 1	to	1.5	
			20%: 1.5	to	5	
			5%: 5	to	25	
Absorber Pressure Drop, psi/ft bed ht.	0.4					
Absorption Cycle, hrs	30					
Max. Vessel Dia, ft	12.5					
Max Vessel Ht., ft	37.5					
GAS TURBINE						
Pressure Ratio	13.5					
Turbine Inlet T., °F	2,300					
Exhaust Flow, lb/s	938					
Thermal NO_x, frac. air N fixated $\times 10^{-5}$	4.25	U	1.0	to	7.5	
Fuel NO_x, % conv. of NH_3 to NO_x	90	T	50	to	100	(90)
Converted CO, wt-% CO in fuel gas	98.85	U	97.72	to	99.99	
SELECTIVE CATALYTIC REDUCTION						
NO_x Removal, %	80					
Temp., °F	717					
No. Cat. Layers	3					
Layer Replacement Interval, hours	11,388	U	5,694	to	17,082	
NH_3 Slip, ppmv	10	U	10	to	20	
Catalyst Activity Uncertainty Factor‖	0.5	U	0	to	1	
Dilution Steam Ratio, H_2O/NH_3	19					
Pressure Drop, psi	4.0	U	1.9	to	6.1	

†Det. Value = Deterministic or nominal (best guess) value.

‡ Five columns are shown to define probability distributions. The first indicates the type of distribution, where F=Fractile distribution; N=Normal distribution; T=Triangular distribution; U=Uniform distribution. The remaining four columns provide the parameters of the distributions. For Uniform distributions, the lower and upper bounds are given. For the triangular distribution, the mode is given in parentheses. For the fractile distribution, the lower and upper bounds for each range are given, along with the probability of

DESCRIPTION AND UNITS	DET.† VALUE	DISTRIBUTIONS AND THEIR PARAMETERS‡				
CAPITAL COST PARAMETERS (fractions)						
Engineering and Home Office Fees	0.10	T	0.07	to	0.13	(0.10)
Indirect Construct. Cost Factor	0.20	T	0.15	to	0.25	(0.20)
Project Unc.	0.175	U	0.10	to	0.25	
General Facilities	0.20					
DIRECT COST CONTINGENCIES AND UNCERTAINTIES (% of estimated direct cost) §						
Coal Handling	5					
Limestone Hdlg.	5					
Oxidant Feed	10					
Gasification	20	T	0	to	40	(20)
Sulfation	40	T	20	to	60	(40)
Zinc Ferrite	40	U	0	to	80	
Sulfuric Acid Plant	10					
Boiler Feedwater	0					
Gas Turbine	25	U	0	to	50	
HRSG	2.5					
SCR	10	T	0	to	20	(10)
Steam Turbine	2.5					
General Facilities	5	U	0	to	10	
MAINTENANCE COSTS (% of process area total cost)¶						
Coal Handling	3					
Limestone Hdlg.	3					
Oxidant Feed	2					
Gasification	4.5	T	3	to	6	(4.5)
Sulfation	4	T	3	to	6	(4)
Zinc Ferrite	3	T	3	to	6	(3)
Boiler Feedwater	0					
Gas Turbine	2	T	1.5	to	6	(2)
HRSG	1.5					
SCR	2.0	T	1.5	to	3	(2)
Steam Turbine	1.5					
General Facilities	1.5					
OTHER FIXED OPERATING COST PARAMETERS						
Labor Rate, $/hour	19.70	N	17.70	to	21.70	(19.70)
VARIABLE OPERATING COST PARAMETERS						
Limestone, $/ton	18	T	18	to	25	(18)
Zinc Ferrite, $/lb	3.00	T	0.75	to	5.00	(3.00)
SCR Catalyst, $\$/ft^3$	250	U	250	to	840	
Ammonia, $/ton	150	U	150	to	225	
Ash Disposal, $/ton	10	T	10	to	25	(10)
DIRECT COST REGRESSION MODEL ERROR TERMS ($ million)						
HRSG	0	N	-17.3	to	17.3	(0)
SCR	0	N	-0.13	to	0.13	(0)
Steam Turbine	0	N	-15.8	to	15.8	(0)

Table 1. Footnotes (Continued)

sampling within that range. For normal and lognormal distributions, the 99.8 percent probability range is given. For normal distributions, the mean is shown in parentheses in the last column.

§ For direct costs, the deterministic values represent "contingency factors" as defined by EPRI and others.[25] For probabilistic studies, uncertainty in capital cost is represented by an uncertainty factor, which is described by a probability distribution.

¶ Includes indirect capital costs and contingency costs prorated to each process area

‖ Catalyst activity is caculated as follows:

$$A(t) = A_{min} + A_{inc} \exp\left(-\frac{t}{\tau_a}\right)$$

See Frey for details.[22] The uncertainty factor is used to calculate A_{min}:

$$A_{min} = 0.5 + 0.4\ f_u$$

and to calculate t_a based on a reference activity level $A(t_1)$:

$$A(t_1) = 0.75 + 0.2\ f_u;\ t_1 = 8760 \text{ hours}$$

where $A(t)$ = relative catalyst activity, t = time, A_{min} = minimum catalyst activity, A_{inc} = incremental activity loss over time, t_a = activity loss time constant, f_u = uncertainty factor.

Table 2. Summary of results from deterministic and probabilistic simulations of a 730 MW air-blown KRW gasifier-based IGCC system with hot-gas cleanup and SCR.†

Parameter‡	Units§	Deter. Value¶	Median $f_{0.50}$	Mean μ	Std Dev σ	Range $f_{0.05}$ to $f_{0.95}$
Plant Performance						
Thermal Efficiency	%, HHV	40.9	41.0	40.9	0.5	39.9 - 41.7
Coal Consumption	lb/kWh	0.743	0.741	0.743	0.009	0.727 - 0.760
Process Water Cons.	lb/kWh	0.768	0.768	0.768	0.015	0.742 - 0.793
Plant Discharges						
SO_2 Emissions	lb/10^6 Btu	0.013	0.014	0.014	0.001	0.013 - 0.016
NO_x Emissions	lb/10^6 Btu	0.148	0.104	0.104	0.028	0.058 - 0.147
CO Emissions	lb/kWh	0.005	0.005	0.005	0.003	0.005 - 0.009
CO_2 Emissions	lb/kWh	1.72	1.71	1.72	0.021	1.69 - 1.76
Solid Waste	lb/kWh	0.230	0.228	0.228	0.012	0.205 - 0.247
Plant Costs						
Total Capital Cost	$/kW	1,535	1,530	1,527	79	1,408 - 1,653
Fixed Operating Costs	$/kW-yr	51.4	54.3	54.6	4.6	46.7 - 63.0
Variable Oper. Costs	mills/kWh	19.9	20.8	20.9	0.6	19.9 - 22.0
Coal	mills/kWh	15.3	15.2	15.3	0.2	15.0 - 15.6
Other	mills/kWh	4.7	5.5	5.6	0.6	4.7 - 6.6
Cost of Electricity	mills/kWh	56.8	58.2	58.2	2.1	54.6 - 61.5

† 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.

‡ 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.

§ HHV = higher heating value.

¶ 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

the uncertainties assigned to model input parameters. Model results are given in Table 2 for both deterministic point-value and probabilistic simulations. All results reported here are based on a plant size of approximately 730 MW using Illinois No. 6 coal. A few of these results are discussed in more detail.

Uncertainty in performance and cost

The uncertainty in the plant thermal efficiency covers a 90% probability range of less than 2 percentage points, and the mean, median, and deterministic values approximately coincide. The distribution is slightly skewed toward lower values. This result is expected due to the negative skewness of the uncertainty in carbon conversion. Conversely, the plant heat rate, which is inversely related to plant thermal efficiency, has a slight positive skewness, as illustrated in Fig. 4. While this result shows close agreement between the deterministic

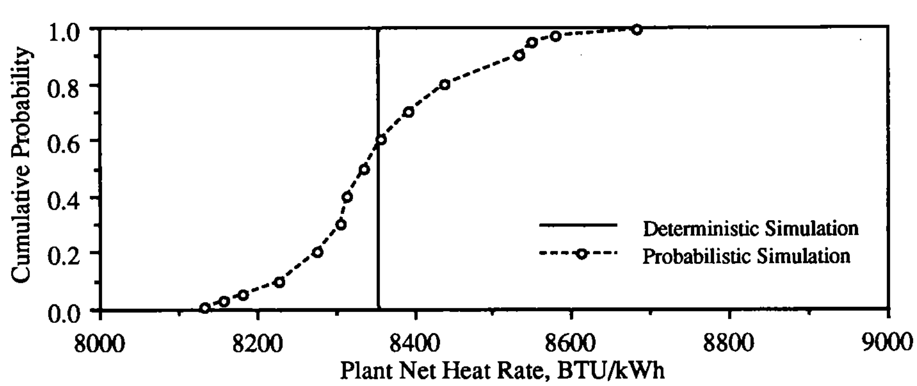

Fig. 4. Comparison of deterministic and probabilistic results for the plant net heat rate.

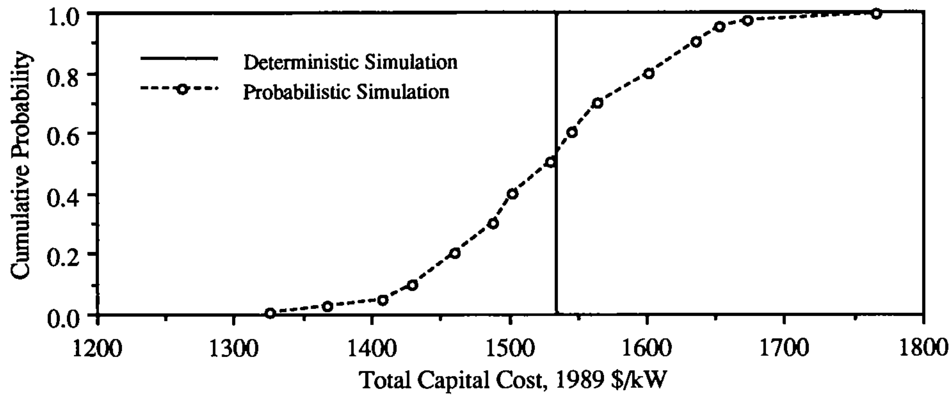

Fig. 5. Comparison of deterministic and probabilistic results for total capital cost.

estimates and the central values from the probabilistic simulation, such findings are not typical of all technologies. For example, for other IGCC systems, the deterministic estimate may substantially over-predict plant efficiency.[1]

The advanced IGCC system with hot-gas cleanup has very low SO_2 emissions compared to conventional coal-fired power plants with flue gas desulfurization.[27] This system, which is equipped with SCR for NO_x control, also has lower NO_x emissions than typical coal-fired power plants. From Table 2, the median NO_x emission rate is lower than the deterministic estimate. This result is obtained because of the negative skewness of the uncertainties in both the formation rate of ammonia in the gasifier and in the conversion rate of fuel-bound nitrogen (ammonia) to NO_x in the gas turbine combustor.

In Fig. 5, the uncertainty in total capital cost is compared to the deterministic estimate. In this case, the deterministic estimate, which includes process and project contingency factors, coincides with the median value of the probabilistic simulation. Thus, there is approximately a 50% chance of cost overrun associated with the deterministic estimate of $1535/kW. Because the performance parameter uncertainties were symmetric or only moderately skewed, and because all of the cost related uncertain parameters affecting capital cost were assumed to be symmetrically distributed, the uncertainty in capital cost is approximately symmetric. The 90% probability range for capital cost is $240/kW, or approximately ±$120/kW from the nominal estimate. This is a relatively narrow range of capital cost uncertainty compared to other technology options. Furthermore, the symmetric nature of the uncertainty for capital cost is not typical of many other advanced technologies, for which there is often greater than a 50% chance of cost over-run.[1,26]

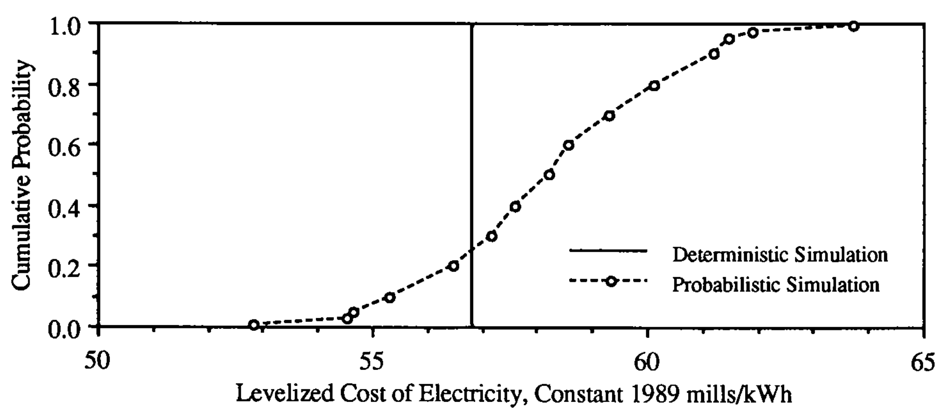

Fig. 6. Comparison of deterministic and probabilistic results for the cost of electricity.

In spite of the agreement between the deterministic and probabilistic results for capital cost, the two analyses do not agree with respect to the cost of electricity, as seen in Fig. 6. There is more than a 75% probability that the cost will be higher than the deterministic estimate. In the probabilistic analysis, the uncertainties in the maintenance cost of the gas turbine, zinc ferrite, sulfation, and SCR process areas were assumed to be positively skewed, reflecting the lack of commercial experience with these systems for this application. Also, the unit costs of limestone, zinc ferrite sorbent, SCR catalyst, and ash disposal were assumed to be positively skewed, representing uncertainties in market conditions and environmental regulations. These assumptions affect fixed and variable operating cost and, in turn, the cost of electricity.

Key uncertainties

The primary advantage of probabilistic simulation over traditional sensitivity analysis is the *simultaneous* incorporation of uncertainties in multiple model inputs. The resulting interactions among uncertain variables results in uncertainties in measures of process viability. Research can provide additional information about the uncertain input variables, resulting in changes in their uncertainty distributions (such as the mean or standard deviation) and, in turn, in the overall uncertainties of the technology. Therefore, it may be fruitful to reduce the uncertainties of key variables that contribute most to the risk of technology failure.

The key input uncertainties resulting in uncertainty in plant efficiency, total capital cost, and the cost of electricity are shown in Table 3. These results are based on partial correlation coefficient analysis.

The plant efficiency is most strongly influenced by uncertainty in the gasifier carbon conversion efficiency. However, uncertainties related to the sulfation unit are also significantly correlated with efficiency. In the air-blown KRW system, limestone is used as a sorbent to

Table 3. Key uncertainties for air-blown KRW-based IGCC based on partial correlation coefficients.

Rank Order	Selected Output Parameter†‡					
	Efficiency		Total Capital Cost		Levelized Cost of Electricity	
	Correlated Input Parameters	PCC	Correlated Input Parameters	PCC	Correlated Input Parameters	PCC
1	Gasifier Carbon Conversion	0.999	Project Uncertainty	0.999	Project Uncertainty	0.998
2	CaS Sulfation Rate	0.998	Gas Turbine Direct Cost	0.999	Gas Turbine Direct Cost	0.996
3	Gas. Oxygen/Carbon Ratio	-0.996	Gasification Direct Cost	0.998	Gasification Direct Cost	0.995
4	Gasifier Temperature	0.987	Indirect Construction Cost	0.998	Indirect Construction Cost	0.991
5	Gas Turbine CO Conversion	0.972	Std. Error HRSG Model	0.996	Gas Turbine Maintenance	0.990
6	Gasifier Ammonia Yield	0.913	Std. Error Steam Turbine	0.995	Gasification Maintenance	0.986
7	Gasifier Ca/S Ratio	0.826	Eng'r & Home Office Fees	0.995	Ash Disposal Unit Cost	0.982
8	Sulfator Carbon Conversion	0.757	CaS Sulfation Rate	-0.969	Std. Error HRSG Model	0.980
9	Gas Turbine Thermal NO_x	-0.659	Sulfation Direct Cost	0.967	Eng'r & Home Office Fees	0.980
10	Gas Turbine Fuel NO_x	-0.639	General Facilities Dir. Cost	0.966	Std. Error Steam Turbine	0.976
11	Gasifier Sulfur Capture	0.560	Zinc Ferrite Unit Cost	0.965	CaS Sulfation Rate	-0.970
12			Zinc Ferrite Direct Cost	0.958	Gasifier Ca/S Ratio	0.968
13			SCR Catalyst Unit Cost	0.953	SCR Catalyst Unit Cost	0.955
14			Gasifier Carbon Conversion	0.951	Zinc Ferrite Unit Cost	0.941
15			Gasifier Ammonia Yield	0.909	Limestone Unit Cost	0.928
16			Gasifier Ca/S Ratio	0.906	Gasifier Ammonia Yield	0.905
17			Gasifier Temperature	-0.782	Sulfation Direct Cost	0.896
18			Gas Turbine Thermal NO_x	0.698	Sulfation Maintenance Cost	0.851
19			SCR Replacement Interval	0.543	General Facilities Dir. Cost	0.843
20			Gas Turbine Fuel NO_x	0.529	Gas. Oxygen/Carbon Ratio	0.841

† 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 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; Eng'r = Engineering; Dir. = Direct; SCR = selective catalytic reduction; Gas. = Gasifier.

‡ Only results that are statistically significant are shown, up through the 20th most sensitive input uncertainty. For plant efficiency, correlation coefficients after the 11th most important are not statistically significant.

remove sulfur during gasification. Because of the reducing atmosphere in the gasifier, the spent sorbent contains sulfur in the form of calcium sulfide. The calcium sulfide must oxidize to calcium sulfate in a fluidized bed boiler prior to landfilling the spent sorbent. A high sulfide concentration would result in a solid waste which would be classified as hazardous under RCRA. However, the conversion rate of calcium sulfide to calcium sulfate in the boiler is uncertain. The energy released from this exothermic reaction is used to generate steam for the plant steam cycle, and is thus recovered as an energy credit.

The total capital cost is strongly influenced by uncertainties in indirect capital costs, process area direct costs, and the error terms of two direct cost regression models.[1] For this technology, uncertainty in capital cost is not strongly influenced by performance uncertainties. Similarly, uncertainty in the cost of electricity is influenced primarily by capital, fixed operating, and variable operating cost uncertainties, with weaker influences from performance-related uncertainties. Of the skewed uncertainties affecting the cost of electricity, the gas turbine and gasifier maintenance costs are the most highly correlated. The ash disposal, SCR catalyst, zinc ferrite sorbent, and limestone unit costs are also significantly correlated.

Many of the key uncertainties identified here, such as carbon conversion efficiency and maintenance costs, can be addressed by targeted research and development efforts.

Probabilistic sensitivity analysis

Another approach to identifying key uncertainties is probabilistic sensitivity analysis. Insight into the sensitivity of output variable uncertainties to the assumptions regarding uncertainties in input variables can be obtained by comparing the effect that different assumptions have on the result. One type of useful insight is the relative importance of uncertainties in performance parameters versus cost parameters. Another is the relative contribution to uncertainty from different process areas. Through probabilistic sensitivity analysis, it is possible to characterize the effect that specific uncertainties or groups of uncertainties have on a given output variable. In cases where uncertainties are excluded from a case study, the probability distribution for the parameter is replaced by its deterministic value.

An example of a probabilistic sensitivity analysis is shown in Fig. 7 for the cost of electricity. The range of uncertainty in the cost of electricity solely attributable to uncertain performance-related parameters is narrow. The 90% probability range attributable to performance only is less than 2 mills/kWh, from 55.4 to 56.9 mills/kWh. Uncertainties in capital cost are shown to substantially increase the variance in the cost of electricity without shifting the central value of the distribution significantly. The 90% probability range in this case covers 5.8 mills/kWh from 53.4 to 59.2 mills/kWh.

The interaction between uncertainty in O&M costs with performance uncertainties results in an upward shift in the central value of almost 2 mills/kWh and an increase in the variance. As

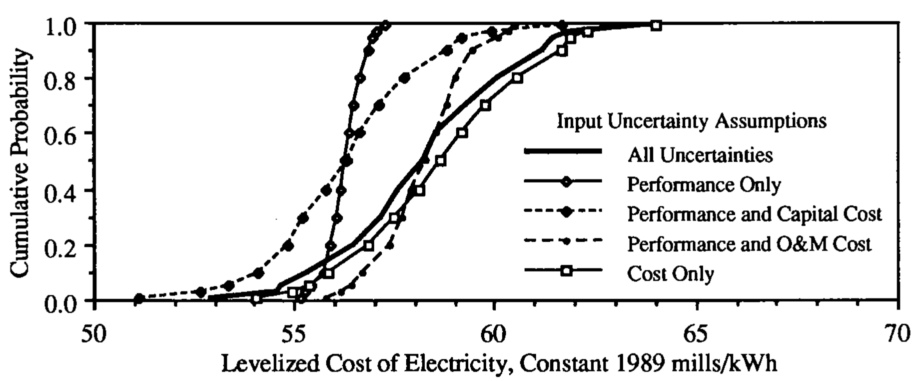

Fig. 7. Sources of uncertainty for the cost of electricity.

seen in Fig. 7, the difference between the case with uncertainties in performance and O&M costs and the "all uncertainties" case is in the variance, not the median. The difference between these two is the inclusion of the symmetric capital cost uncertainties in the "all uncertainties" case. When all performance parameters are held at their deterministic "best guess" values, and all cost-related uncertainties are included in the probabilistic simulation, the result is very similar to that obtained when all uncertainties are simulated.

Thus, from the probabilistic sensitivity analysis, it is clear that performance-related uncertainties are a relatively minor component of overall uncertainty in cost for this technology. Furthermore, while the variance in the result is strongly influenced by uncertainties in capital cost, it is the uncertainties in O&M costs that are responsible for the shift in the central tendency of the distribution for the cost of electricity. Therefore, the risks of cost growth for this particular technology are shown to be embodied in the annual operating and maintenance costs. Uncertainties in O&M costs are often overlooked in conceptual design studies, which tend to focus more on capital costs. This is especially true when developing estimates of contingencies costs.

Comparing designs probabilistically

An example of probabilistic design analysis is considered here. The design assumption concerns whether an SCR NO_x control system is employed. Such a system is likely to be required to meet local environmental permitting requirements in some regions of the U.S. To evaluate the effect of SCR on the IGCC system, two probabilistic simulations were executed: one with SCR (the base case) and one without. 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 impact of the SCR system on selected measures of plant performance, emissions, and cost is summarized in Table 4, based on both deterministic and probabilistic simulations. The SCR system increases the plant heat rate (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. The heat rate penalty estimated from the deterministic simulations is substantially higher than the range estimated from the probabilistic simulations. This is due to the negative skewness of uncertainties in the uncontrolled NO_x emission rate, which in turn influences the

Table 4. Impact of SCR on the performance, emissions, and cost of a 730 MW air-blown KRW-based IGCC system with hot-gas cleanup.†

Parameter	Units	Deter. Value‡	Median $f_{0.50}$	Mean μ	Std Dev σ	Range $f_{0.05}$ to $f_{0.95}$
Plant Performance						
Change in Heat Rate	BTU/kWh	48	23	24	6.3	14 - 33
Plant Discharges						
NO_x Emissions	lb/10^6 Btu	0.56	0.39	0.38	0.11	0.20 - 0.55
NH_3 Emissions	lb/10^9 Btu	9.97	14.8	14.8	2.9	10.6 - 19.2
SCR Costs						
Total Capital Cost	$/kW	44	44	44	7	34 - 57
Fixed Operating Costs	$/kW-yr	0.8	0.6	0.6	0.1	0.4 - 0.7
Variable Oper. Costs	mills/kWh	0.5	0.7	0.7	0.2	0.3 - 1.1
Cost of Electricity	mills/kWh	1.4	1.6	1.6	0.3	1.1 - 2.1

† All values shown are differences between a system with SCR and one without SCR. 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.

‡ 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

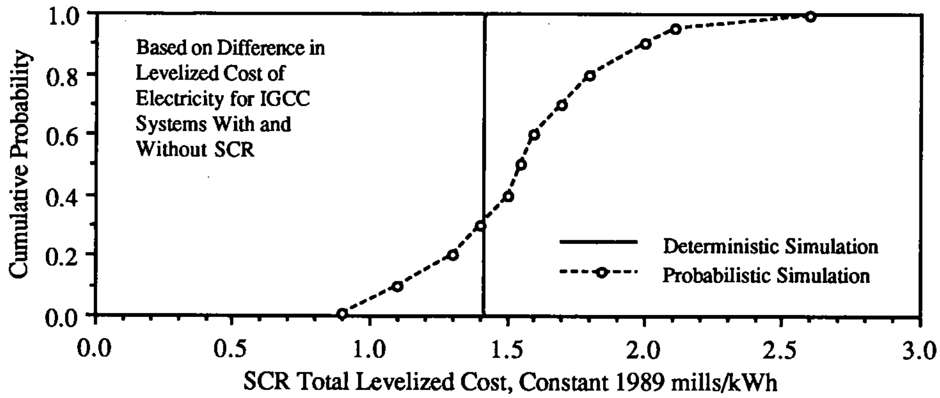

Fig. 8. Comparison of deterministic and probabilistic estimates of the levelized total cost for selective catalytic reduction NO_x control.

ammonia injection requirement, steam requirement, and auxiliary electric power consumption. This skewness also results in a higher estimate of NO_x emission reduction from the deterministic simulation than from the probabilistic simulations.

A pollutant of potential concern is ammonia. A portion of ammonia passes through the SCR system unreacted, and is vented to the atmosphere. Many design studies assume that this ammonia "slip" may be approximately 10 ppm, and thus this value was used as the "best guess" in the deterministic simulation. However, values up to 20 ppm are not uncommon.[28] Thus, the deterministic estimate is at the low end of the range of probabilistic results. For the IGCC system without SCR, ammonia is assumed not to be emitted.

The capital cost associated with the SCR system is uncertain by a factor of 1.7, due primarily to uncertainties affecting catalyst requirement and to uncertainty in the catalyst unit cost. A comparison of the deterministic and probabilistic estimates of the levelized total cost of the SCR system is shown in Fig. 8. The disparity between the estimates is due primarily to uncertainty in the unit cost of the catalyst. There is a 70% probability that the levelized cost will be higher than the "best guess" estimate. Furthermore, the total levelized cost is uncertain by a factor of nearly 2 over the 90% probability range.

Thus, while the SCR system will substantially reduce the NO_x emissions of the IGCC system, it has associated problems due to ammonia emissions and catalyst disposal, and it is likely to increase the capital cost by approximately $44/kW and levelized cost by 1.6 mill/kWh. It may increase levelized costs by as much as 2.5 mills/kWh. In this example, deterministic estimates of both capital and levelized cost are lower than the central values from the probabilistic estimates. However, without SCR, and in lieu of other NO_x control measures such as advanced rich/lean or catalytic combustors, the NO_x emissions from this IGCC system are likely to be unacceptably high.

Analysis of design trade-offs probabilistically thus provides explicit insights into the risks of potentially high cost or potential poor performance associated with specific options. Other examples of this type of analysis are reported by Frey[1] and Frey and Rubin.[26,29]

OTHER APPLICATIONS

Other applications of the probabilistic evaluation method not discussed here include: (1) evaluation of the reductions in uncertainty that may be obtained from further process research; (2) evaluation of alternative judgments regarding model parameter uncertainties by different experts as they affect model results; (3) evaluation of the importance of correlation structures in model parameter uncertainties; (4) comparative analysis of competing technologies under uncertainty; and (5) the use of decision analysis techniques to interpret modeling results. These types of applications are discussed elsewhere.[1]

DISCUSSION AND CONCLUSIONS

A new capability for stochastic analysis has been developed for the ASPEN chemical process simulator. This capability can be applied to analyse uncertainties in any process that can be modeled using ASPEN. A detailed case study has been presented to illustrate the application of the capability and the types of results that may be obtained.

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.

As shown in many of the case studies, the influence of skewed distributions on model results can be important. Skewness in model input parameters tends to shift the central tendency of performance and cost results, and can lead to distributions with long tails representing unfavorable outcomes. These types of interactions cannot be evaluated systematically in deterministic analysis. While the information requirements for probabilistic analysis may be more demanding, the estimates of performance and cost are likely to be more realistic. Thinking about uncertainties is an important way to gain understanding into the key factors that drive the risk of failure or likelihood of success.

Thus, while traditional approaches to technology evaluation inadequately account for uncertainties and often lead to over-optimistic estimates of performance and cost, the probabilistic evaluation method advanced here permits the effect of uncertainties to be evaluated systematically. Furthermore, many of the "surprises" that often account for "cost growth" can be captured by the use of sufficiently detailed engineering models coupled with specification of uncertainties in specific model parameters. Probabilistic modeling is an important and versatile technique for developing realistic estimates of process viability and for prioritizing further research.

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