PROCEEDINGS

Sixth Annual International
PITTSBURGH
COAL CONFERENCE

September 25-29, 1989
Pittsburgh, Pennsylvania, U.S.A.

Volume 2

(Session 19—Poster Board 2)

Hosted by:
University of Pittsburgh

School of Engineering
Department of Chemical & Petroleum Engineering

NO. U.S. 37 STOCHASTIC MODELING OF INTEGRATED COAL GASIFICATION COMBINED CYCLE SYSTEMS USING ASPEN

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ABSTRACT

IGCC power systems represent a promising new approach for the clean and efficient use of coal for power generation. At the present time, however, there is still limited experience with IGCC systems on a commercial scale. The uncertain nature of the limited performance and cost data for the first generation systems, coupled with uncertainties associated with alternative process configurations, suggests a strong need for systematic analysis of uncertainty in evaluating alternative designs or concepts. In this paper, a probabilistic modeling system is described which provides the capability for analysis and decision making in the face of uncertainties. IGCC systems are currently modeled using ASPEN, a steady state simulator. A stochastic modeling capability has been added to the public version of ASPEN. This new capability is illustrated for a specific IGCC flowsheet.

1. INTRODUCTION

There is significant interest today in the ability of integrated coal gasification combined cycle (IGCC) systems to provide electricity reliably and at lower cost relative to conventional fossil fuel alternatives. The ability of IGCC systems to meet stringent environmental emission standards is another extremely attractive feature of this technology. Thus, intensive research, development, and demonstration projects are currently underway to develop improved, lower cost technology for IGCC systems.

In addition to the technical aspects of IGCC technology, there is also a strong need for research to identify the best ways of configuring IGCC plants, and of incorporating advanced cleanup and other technologies into an overall system to produce electricity at minimum cost. Thus, a number of computerized simulation models have been developed to allow IGCC systems to be analyzed using basic mass and energy balance relationships together with performance characteristics of individual system components. However, while computer simulation models have grown in sophistication and complexity, certain capabilities important to R&D planning, system design and economic analysis still remain to be developed.

The focus of this paper is on the limitations of existing models to analyze and display the uncertainties associated with IGCC process performance and cost. The ability to analyze uncertainty is especially important in the context of on-going research and development, where technical and economic parameters for individual processes and overall system designs are not well established. Uncertainties also are important in comparing advanced systems designs with "baseline" systems reflecting currently commercial technology. Here, the probability of achieving significant cost savings or improvements in performance is of special concern, particularly for R&D planning.

2. CONVENTIONAL UNCERTAINTY ANALYSIS

Conventional simulation models typically employ a Fortran code which produces a deterministic (point estimate) result for a particular set of input assumptions. To analyze uncertainty, the capability to perform sensitivity analysis through a series of multiple runs is usually available. Typically, however, only one or two parameters are varied at a time in a simulation framework which may contain a large number of independent variables. Thus, important interactions or cases may be overlooked. Although larger numbers of cases may be run as part of a sensitivity study, the large volume of output that is generated makes results cumbersome or difficult to interpret and/or display. Even where many cases are analyzed, sensitivity analysis provides no information as to the likelihood of different outcomes.

Deterministic performance models of a number of IGCC systems have been developed by the U.S. Department of Energy's Morgantown Energy Research Center (DOE/METC) using the Advanced System for Process Engineering (ASPEN) process simulator (MIT 1989). Predictions about the performance and cost of IGCC systems involve many uncertainties. The METC-enhanced version of ASPEN does have a special case study block plus a Fortran sensitivity block, which can be utilized for sensitivity analyses. The case studies or sensitivity analyses involves running multiple simulations by varying one or more parameters at a time. As noted earlier, this type of analysis is restrictive in that it does not take into consideration the interactions among many of the uncertain model parameters. Further, this approach may result in large quantities of output data and large computer run time.

In contrast, the probabilistic uncertainty analysis framework described in this paper incorporates a number of attributes not found in current IGCC simulation models. This paper describes the current status of a research project initiated in May 1988 to develop a general stochastic simulation framework for analyzing the performance and cost of IGCC systems.

THE STOCHASTIC SIMULATION MODEL

The approach adopted in this research involves adding a stochastic modeling capability for uncertainty analysis to the public version of the DOE/METC ASPEN simulator. This involves two primary tasks: (1) identification of a suitable software environment for performing probabilistic analysis, and (2) implementation of the software in ASPEN.

3.1 The Probabilistic Software Environment

A Fortran program developed by Iman and Shortencarier (1984) was found to be suitable for assigning probabilistic distributions to input variables and performing the sampling. The program uses the Latin Hypercube Sampling (LHS) technique for generating probability distributions. In the LHS method, which is a refinement of Monte Carlo simulation, a distribution is divided into intervals of equal probability, and samples are taken at random from within each interval. LHS guarantees that values from the entire range of a distribution are sampled in proportion to the probability density of that distribution, whereas the traditional Monte Carlo method samples random points in the distribution. Because parameter input distributions are sampled over the entire range of probable values, the number of samples required to adequately represent a distribution is much smaller than for Monte Carlo simulations. Thus, LHS significantly reduces the computational effort required for a probabilistic analysis.

The Iman and Shortencarier program has been implemented in ASPEN for sampling input parameters. The software provides a set of eight types of probability distributions for characterizing input variables (normal, lognormal, uniform, loguniform, modified uniform, modified loguniform, beta, and triangular). There is also the ability to specify any user-defined distribution.

Once a set of runs has been made, the resulting output variables must be analyzed. Several statistical packages were surveyed to identify the most suitable for output analysis. The basic capability needed for probabilistic analysis is the construction of a probability density function (PDF) and a continuous distribution function (CDF). A new stochastic unit operation block has been implemented which provides the user with histograms and scatter plots of PDFs and CDFs for model output variables. In addition to this, a program developed by Iman, Shortencarier and Johnson (1985) has been utilized to quantify the sensitivity of an output result to each of the uncertain inputs. This method allows an estimate to be made of which input uncertainties are the most significant contributors to the uncertainty in a given output. The methods available for measuring the sensitivity of outputs to inputs include partial correlation coefficients (PCC) and standardized regression coefficients (SRC) for linear correlations, plus partial rank correlation coefficients (PRCC) and standardized rank regression coefficients (SRCC) for nonlinear correlations.

Standardized regression coefficients (SRC/SRCC) can be used to measure the relative contribution of the input variables to the uncertainty of the output variables. This analysis involves standardization of all distributions and a multivariate regression of an output variable based on the input variables. The regression coefficients for each input variate then indicate the relative importance of that factor on the output result. A correlation coefficient is also calculated to measure how well the regression equation fits the data.

A partial correlation coefficient analysis is used to identify the degree of linearity in correlations between output and input variables. Partial correlations measure the unshared contribution of each input variable to the output, whereas standardized correlations measure the shared contribution of the input to the output. These measures are related, but provide different insights as to the sources of uncertainty.

3.2. Implementation in ASPEN

To implement the stochastic modeling capability, ASPEN's modular nature (consisting unit operation modules or blocks) has been utilized. A new unit operation block, STOCHA, has been added to the ASPEN unit operation module library. Initially, this new block was added in the form of a user block. More recently it has been added as a permanent unit operation block in ASPEN. The structure of the block and it's use are briefly described below. Details are provided elsewhere (Diwekar 1989).

The unit operation block, STOCHA, characterizes the uncertainty in model input parameters in terms of probability distributions, and analyzes their effect on selected output variables. To link STOCHA to the ASPEN flowsheet, two Fortran blocks are needed. This type of stochastic modeling capability can be used for systematic probabilistic analysis. The stochastic modeling approach involves

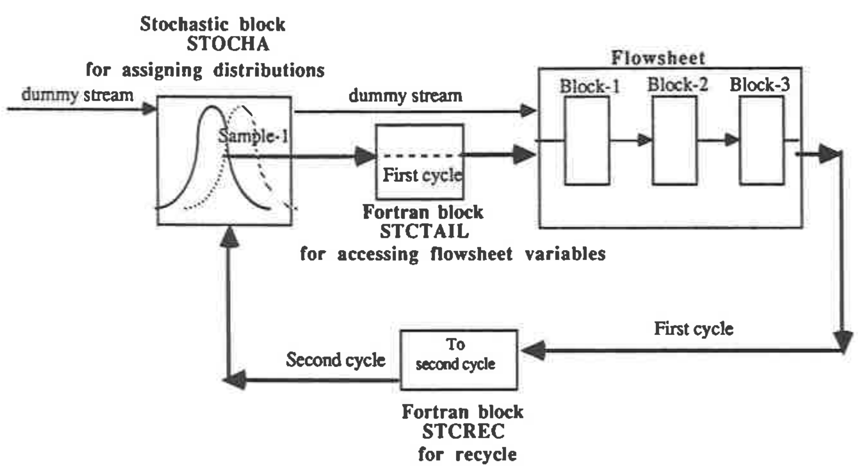
1. Specifying the uncertainties in key input parameters in terms of probability distributions;
2. Sampling the distributions of these parameters in an iterative fashion;
3. Propagating the effects of uncertainties through the process flowsheet; and
4. Applying graphical and statistical techniques to analyze the results.

The stochastic block assigns user-specified distributions to the key input parameters, and then uses Latin Hypercube Sampling (LHS) to pass the sampled values of each uncertain variable to the flowsheet. After a flowsheet simulation is run, the output variables of interest are collected. The simulation is then repeated for a new set of samples selected from the probabilistic input distributions. A new Fortran block is used to control the cycling of the stochastic block, and another Fortran block, called STCTAIL, is used to access and assign samples to model parameters.

After all samples or observations have gone through this cycle for a specified number of times (typically 20 to 100 or more, depending on the accuracy sought by the user), the stochastic block analyzes the output. As indicated earlier, the output options include cumulative and non-cumulative probability density functions of input and output parameters, plus various correlation coefficients which measure the effects of input uncertainties on the output results.

Figure 1 shows the use of the stochastic block for uncertainty analysis of a flowsheet. The cycle for uncertain variables consists of: (a) the stochastic block, STOCHA, for assigning parameter uncertainty distributions; (b) the Fortran block, STCTAIL, for accessing variables and assigning sampled values; and (c) the Fortran recycle block, STCREC, for data output collection and recycling.If there are convergence loops nested within the flowsheet of a stochastic cycle, and if entire flowsheet calculations are involved in the analysis, it may be necessary to use an additional Fortran cycle control block to mark the beginning and end of the convergence cycle. Appropriate software also has been implemented to handle this case, as described (by Diwekar 1989).

Figure 1. Basic Operation of the Stochastic Simulation Method



4. AN ILLUSTRATIVE EXAMPLE

The performance models developed by METC for IGCC systems include different gasifier designs and gas stream cleanup systems. Present METC models consists of fixed bed, fluidized bed and entrained bed gasifiers, plus cold gas and hot gas cleanup systems (Stone 1985).

The ASPEN IGCC models typically consist of approximately 80 unit operation blocks and eight flowsheet sections. While the bulk of the models are comprised of generalized unit operation blocks (e.g., pumps, heat exchangers, pressure vessels, etc.), there are a number of Fortran blocks and design specification blocks which are specific to IGCC systems or to a particular flowsheet. There are also user-specified models to handle coal properties, and a Fortran block used as a summary report writer to concisely present plant performance results.

The following paragraphs illustrate the use of the probabilistic modeling capability using the KRW IGCC process model, which is of interest for on-going studies.

4.1 The KRW Fluidized-Bed IGCC System

DOE/METC has developed a simulation model based on a conceptual design of a commercial IGCC plant using the Kellogg-Rust-Westinghouse (KRW) ash agglomerating pressurized fluid-bed gasifier with conventional cold gas cleanup processes (Bechtel 1983). ASPEN performs a steady-state computer simulation of this process. The simulation flowsheet contains 83 unit operation blocks (i.e., models of unit operations such as pumps, reactors, and compressors), plus user routines to calculate ash enthalpy and coal decomposition. The eight plant sections which are simulated are Gasification, Solids Separation, Gas Cleaning and Cooling, Gas Turbine, Effluent Water Primary Treatment System, Claus Plant, Beavon-Stretford Unit, and the Steam Cycle.

The KRW-IGCC simulation model was developed by to provide accurate mass and energy balances, and to track major environmental species (SOx, NOx, and particulates). The overall simulation runs in 81.3 seconds of CPU time on a Vax-3200 computer workstation. Table 1 shows a summary of results obtained for a case study of a 130 MW system using deterministic input parameters (Stone 1985).

4.2 Stochastic Simulation of the KRW IGCC System

There are large number of input variables in a flowsheet whose values may be uncertain. There are also certain design specifications which may vary according to conditions. The stochastic modelling capability can be used to study the effect of these variabilities or uncertainties on plant performance.

To illustrate the stochastic modelling capability for ASPEN, five input variables in the KRW flowsheet are treated as uncertain. Table 2 shows the deterministic values of these parameters as well as the assumed uncertainties given as probability distributions. The decision about which parameters to treat as uncertain, and what type of distribution to apply, depends upon the purpose of the analysis, the data available for use, and the judgment or experience of the analyst. A normal distribution reflects a symmetric but varying probability of a parameter value being above or below the mean value. For a uniform distribution there is an equal likelihood of a value lying anywhere within a specified range, while for a lognormal or triangular distribution there is a higher probability of values lying one side of the median than other. A Beta distribution, on the other hand, is versatile and can have many

TABLE 1. KRW FLUIDIZED-BED IGCC POWER PLANT SYSTEM SUMMARY (from Stone 1985)

*** GASIFIER CONDITIONS ***
Coal Flow Rate: 0.112497E+06 lbs/hr
Oxygen Flow Rate: 0.596235E+05 lbs/hr
Steam Flow Rate: 0.523112E+05 lbs/hr
Gasifier Pressure: 415.0 psia
Gasifier Temperature: 1800 F

*** MS7000 GAS TURBINE CONDITIONS ***
Fuel Flow Rate: 0.158369E+06 lbs/hr
Air Flow Rate: 0.215996E+07 lbs/hr
Steam Flow Rate: 0.475107E+05 lbs/hr
Fuel LHV: 5639.1 Btu/lb, 301.1 Btu/scf
Fuel HHV: 6073.0 Btu/lb, 324.3 Btu/scf
Firing Temperature: 2150.0 F
Combustor Exit Temperature: 2240.7 F
Turbine Exhaust Temperature: 1062.5 F
Thermal Efficiency (LHV) : 0.3416
Generator Efficiency: 0.9850

*** STEAM TURBINE CONDITIONS ***
Superheated Steam Flow Rate: 0.349062E+06 lbs/hr
Superheated Steam Temperature: 986.0 F
Expanded Steam Quality: 0.8770
Generator Efficiency: 0.9850

*** POWER PRODUCTION SUMMARY ***
Gas Turbine: 0.894078E+08 Watts
Steam Turbine: 0.525229E+08 Watts
Compressors: -0.157462E+06 Watts
Pumps: -0.820484E+06 Watts
Oxygen Plant: -0.110834E+08 Watts
Plant Total: 0.129869E+09 Watts

****
PLANT THERMAL EFFICIENCY (HHV) = 0.3900
****

different shapes depending on the two shape parameters that are assigned.

The distributions assigned to the variables in Table 2 are mostly based on the data available from different literature sources and reflects the variability and judgments of different design teams in selecting the values of design parameters for similar systems. For this example, most of the input parameters have been assigned a skewed triangular distribution while the uncertainty of one out of the five parameters is represented by uniform distribution.

TABLE 2. ASSUMED UNCERTAINTY IN MODEL INPUT PARAMETERS

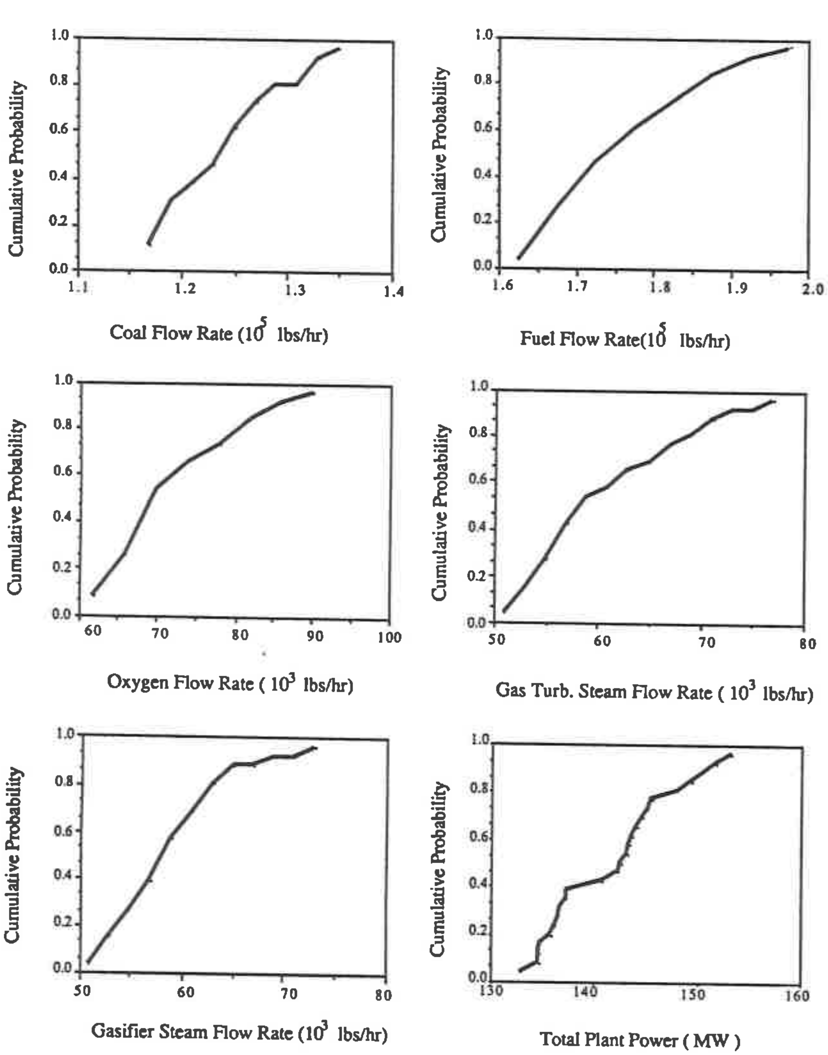
Parameter	Units	Nominal Value	Distribution	Range (Mode)
Oxygen/Coal Ratio	lbs oxidant/lb coal	0.53	Triangular	0.53 - 0.70 (0.53)
Steam/Coal Ratio	lbs steam/lb coal	0.465	Triangular	0.40 - 0.58 (0.47)
Raw Gas Cooler Outlet Temperature	degrees F	335	Triangular	335 - 420 (335)
Gas Turbine Firing Temperature	degrees F	2150	Uniform	2150 - 2300
NOx Steam/Fuel Ratio	lbs steam/lb fuel	0.30	Triangular	0.30 - 0.43 (0.30)

The effect of these uncertainties on selected model output parameters is shown in Figures 2 and 3 in the form of cumulative probability distributions (CDFs) based on 25 samples. The information obtained from the distribution curves and associated statistical data (not shown here) can provide insights not available from conventional deterministic analyses. For example, what is the range of uncertainty of the output variable of interest? What is the most likely value? What range is encompassed by, say, a 90 percent confidence interval? What are the chances that the value will be below or above some certain level?

For the KRW IGCC flowsheet, Figure 2 shows the joint contribution of all five parameter uncertainties on several selected output parameters. Figure 3 further shows the effect of a single parameter uncertainty (gas cooler temperature) versus the combined effect of uncertainties in all five parameters on the total plant efficiency. Overall, it can be seen that there is 5% chance that the value of efficiency is below 37.7 % or above 39.6% , the median being 38.7%. For the range of parameter values used here, the effect of gas cooler temperature alone is seen to be negligible. With only this parameter uncertain the predicted efficiency is the same as the deterministic value (i.e., 39.0%). The overall probabilistic result also shows only a 25% chance of achieving the expected (deterministic) performance. Combinations of input parameter values leading to high thermal efficiency can be found from a more detailed examination of the probabilistic results. Thus, where such parameters are independent (as assumed for this example), a probabilistic analysis also can help identify globally optimum conditions for IGCC system designs. The effects of parameter correlation structures also can be incorporated in an analysis.

Apart from uncertainty analysis results the stochastic modelling framework also displays the effect of different input variables on the output in terms of correlation coefficients. For example, the sensitivity of the coal flow rate based on the correlation coefficients found for this case study in descending order of importance, are: (1) oxygen / coal ratio, (2) combustor temperature, (3) NOx control steam/ fuel gas, (4) steam/coal ratio, (5) raw gas cooler temperature.

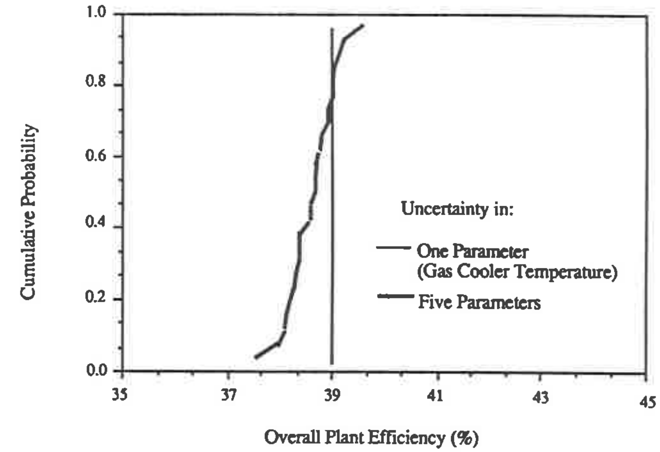
Figure 2. Probabilistic Output Results for KRW IGCC Flowsheet



5. CONCLUSIONS AND FUTURE PLANS

This paper has described a new stochastic modeling capability for the ASPEN chemical process simulator. The stochastic modeling capability can be used to evaluate the performance of any chemical plant which can be formulated using the simulator. An application of this capability to the KRW IGCC system performance model also was illustrated.

Figure 3. Uncertainty in Overall Plant Efficiency



In the future, cost models for selected IGCC systems also will be developed. These models will reflect the capital cost of various plant sections, as well as system operating and maintenance costs. The economic models will be sensitive to key system flow rates and design parameters, and will be fully integrated with the performance models. The cost models can be used to quantify differences in system designs and to identify key uncertainties important for comparative evaluations and research planning. There are three general areas of uncertainty that will be explicitly reflected in the IGCC cost models. These are uncertainties in: (1) process performance parameters (e.g., flow rates, temperatures, pressures, etc.), (2) process area capital costs, and (3) raw material and other system operating costs.

One application of a probabilistic analysis combining uncertainties in performance and cost parameters is in the estimation of a process "contingency factor." A contingency cost is used in traditional cost analyses to represent additional costs that are expected to occur, but that are not included explicitly in the cost estimate. (Indeed, a better name would be "miscellaneous costs."). Typically, this is one of the largest items in an IGCC cost analysis. Process contingency factors are usually estimated as a simple multiplier of nominal process area costs, often based on a "rule-of-thumb" depending on the level of detail of the cost estimate.

One major development sought in this research is the use of probabilistic modeling to refine or replace the simple contingency cost multipliers now commonly employed for economic analyses. A probabilistic modeling approach supplants the traditional contingency factor approach by incorporating expert knowledge about uncertainties at a more disaggregated level (e.g., for specific process performance or cost parameters). Unlike conventional contingency factor estimates, which are applied toward the end of an analysis (e.g., after process area costs have been estimated without regard to their uncertainty), uncertainty estimates using probabilistic methods are developed as an integral part of the analysis.

Furthermore, while simple contingency factors provide no explicit insights into the specific performance or cost parameters that contribute most to the process technical and economic risks, a probabilistic approach permits identification and ranking of the uncertain parameters that contribute most to the overall uncertainty. In this context, a probabilistic approach also can be helpful for identifying research and development priorities that contribute most to cost reductions. In a later phase of this research, judgments regarding key uncertainties in process performance and economic parameters will be elicited in the context of more detailed case studies of probabilistic modeling for IGCC systems.

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