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# A NEW APPROACH FOR IGCC PROCESS SYNTHESIS UNDER UNCERTAINTY

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## ABSTRACT

As the complexity of chemical and energy technologies has increased, the need has grown for new computer-aided design tools for process synthesis. For technologies in the early stages of development and demonstration, the need to incorporate uncertainties in the process synthesis stage is especially great. This paper presents a new and efficient method, based on stochastic annealing, to identify optimal design configurations from a large number of process alternatives, considering the effects of uncertainty. Case studies of an integrated coal gasification combined cycle (IGCC) power plant are presented to illustrate this method. For this case, the new stochastic synthesis framework reduced computational time by 60% compared to an exhaustive search procedure. Greater efficiencies are expected as the number of process configurations increases.

## INTRODUCTION

Integrated gasification combined cycle (IGCC) systems are an emerging technology for the clean and more efficient use of coal for power generation. Several IGCC designs have been demonstrated on a commercial scale, with other advanced concepts currently in the development and demonstration stages. Of particular interest are improved technologies for the gasification and environmental control sections of an IGCC system, especially systems using hot gas cleanup. Since most components of these advanced IGCC systems are still in the design and development phase, significant uncertainties remain regarding their commercial performance and cost.

The United States Department of Energy (DOE) has developed computer-based performance models for several IGCC systems using the Aspen process simulator (Evans, et al., 1979). These models include different gasifier designs (i.e., fixed-bed, fluidized-bed, and entrained-bed gasifiers), and different gas stream cleanup systems based on hot gas or cold gas cleanup technologies (Stone, 1985). Frey

and Rubin (1992) extended the earlier DOE work to include new process performance models for environmental control systems, as well as capital and operating cost models for several variants of IGCC system designs. These Aspen models typically consist of approximately 80-90 unit operation blocks, and up to eight flowsheet sections involving gasification, gas cleanup, and power generation units. While the bulk of the models are comprised of generalized unit operation blocks (e.g., pumps, heat exchangers, pressure vessels), there are a large number of Fortran blocks and design specification blocks (defined by the input program structure of Aspen) which are specific to IGCC systems, or to a particular flowsheet.

Until now, each of these flowsheets was evaluated separately. As the number of technological options increases, however, an exhaustive search through individual flowsheet simulations to identify an optimal design configuration becomes computationally expensive. Consequently, a systematic, efficient procedure for screening multiple alternatives, and selecting an optimal design configuration, is desirable.

In this paper, the problem of identifying the optimal design configuration of an IGCC system is posed as a process synthesis problem, wherein the alternative technological variants are embedded in one flowsheet — a “superstructure” — from which an optimal configuration is identified. An additional advance is the explicit treatment of uncertainty, in contrast to the traditional deterministic approach to analysis. The presence of uncertainties makes the technology evaluation process a computationally intensive problem. This paper presents an efficient approach for the solution of this real-world large-scale synthesis problem.

## PROCESS SYNTHESIS UNDER UNCERTAINTY

Approaches to process synthesis may be classified into four groups: (1) the thermodynamic approach (Linhoff, 1981), (2) the evolutionary method (Nishida et al., 1981), (3) the hierarchical approach based on intuition and judgment (Douglas, 1988), and (4) the optimization or algorithmic approach (Grossmann, 1985; Friedler et al. 1995; Painton and Diwekar, 1994). These approaches, although different in principle, all provide directions for process synthesis research, and each brings different perspectives and advantages to this field. For example, the hierarchical approach provides improved process understanding and motivates novel problem representations, while the optimization approach can prune a search space of alternative configurations to find the best flowsheet that maximizes or minimizes a target function.

This paper focuses on the optimization approach to process synthesis. This approach is especially amenable to generalization and to interfacing with modern process simulators. The optimizer iteratively determines the discrete and continuous decision variables. Discrete variables denote the existence or absence of specific units in the flowsheet, while continuous variables represent flows, operating conditions, and design parameters for system components. In general, the synthesis problem thus involves two elements: choosing the optimal components of a flowsheet, and optimizing a given flowsheet design.

### Stochastic Simulation Capability

Process models involved in conventional optimization methods are typically deterministic in nature, i.e., all input parameters have a single fixed value, and all model results are similarly single-valued. In this paper we add the dimension of uncertainty. Uncertainties in process design arise in the early stages of development and demonstration because available performance data often are scant, and technical and economic parameters are not well established. Thus, a systematic framework to analyze uncertainties is a key step in improving upon current design capabilities. In conventional simulators or simulation programs, sensitivity analysis via a series of multiple runs is the typical approach used to analyze uncertainty. 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 easily may be overlooked. Even where many cases are analyzed, sensitivity analysis for nonlinear models cannot easily provide information about worst case or best case scenarios. Nor does sensitivity analysis provide any measure of the *likelihood* of different outcomes.

A generalized framework for analyzing uncertainties systematically has been developed around a chemical process simulator in our earlier work (Diwekar and Rubin, 1991). This approach allows for probabilistic modeling of any chemical process flowsheet modeled in a simulator, and overcomes the limitations of sensitivity analysis by providing a generalized treatment of uncertainties. This probabilistic or stochastic modeling procedure involves: (1) specifying the uncertainties in key input parameters in terms of probability distributions; (2) sampling the distribution of the

specified parameter in an iterative fashion; (3) propagating the effects of uncertainties through the process flowsheet; and, (4) applying statistical techniques to analyze the results. A major bottleneck in the stochastic modeling framework, however, is the computational intensity of the recursive sampling.

### Stochastic Optimization Capability

Process optimization under uncertainty adds further complexity since it requires optimization as well as uncertainty analysis. Figure 1 shows the schematic of the stochastic optimization procedure developed for a given flowsheet. The procedure involves two recursive loops: the inner stochastic sampling loop, and the outer process optimization loop. Because each loop involves iteration, it is desirable to reduce the computational intensity and the interactions between the two loops in order to address large-scale synthesis problems.

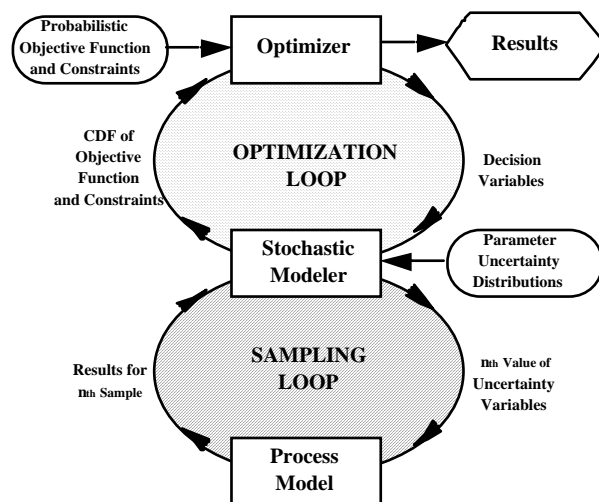


Figure 1. Stochastic Optimization Framework

Recently, a new recursive sampling technique, known as Hammersley sequence sampling (HSS), was shown to exhibit better homogeneity over a multi-variate parameter space compared to conventional sampling methods (Diwekar and Kalagnanam, 1997). In this context, homogeneity is defined as the ability to produce a uniform distribution of points covering the entire sample space, such that the overall distribution is representative of the entire population. Further, it was found that the number of samples required for the HSS technique to converge to different performance measures of a random output variable (e.g., mean, variance or fractiles), subject to input uncertainties, is lower compared to traditional Monte Carlo or Latin hypercube sampling techniques. This rapid convergence property of Hammersley sequence sampling has important implications for stochastic modeling of complex processes. It suggests that precise estimates of any probabilistic function are achievable using a smaller sample size. This efficient sampling method can be used for the inner sampling loop to enhance the computational efficiency of the stochastic optimization framework.

The stochastic annealing algorithm proposed in earlier work (Painton and Diwekar, 1995; Chaudhuri and Diwekar, 1996) is designed to efficiently optimize a probabilistic objective function, and is a good candidate for the outer optimization loop. The algorithm manipulates the sample size automatically, reducing the computational bottleneck of the stochastic optimization problem. This is achieved by augmenting the real objective function with a penalty term that incorporates the error band-width for the probability measure. This algorithm, coupled with the new sampling technique, provides an efficient framework for process synthesis, and optimization under uncertainty.

The optimizer in Figure 1 not only obtains values of the decision variables, but also the number of samples required for the stochastic model. Furthermore, it provides the trade-off between accuracy and efficiency by selecting a larger number of samples as the optimum design is approached. Thus, the stochastic annealing algorithm minimizes central processing unit (CPU) time by balancing the trade-off between computational efficiency and solution accuracy via a penalty term in the objective function. Additional details of the computational method are discussed in Diwekar and Chaudhuri (1997).

### Process Synthesis Capability

To extend the process optimization scheme in Figure 1 to include process synthesis, an additional process “superstructure” is formulated which includes all of the alternative flowsheet structures under consideration. The presence or absence of superstructure components in a particular flowsheet is determined by the flow through each unit, with zero flow indicating the absence of a component. The process synthesis environment then consists of the two loops shown in Figure 2. This new process synthesizer has been linked with the public version of the Aspen process simulator used by DOE.

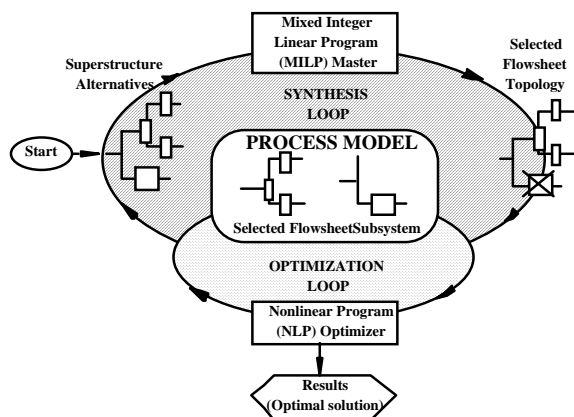


Figure 2. Process Synthesis Framework

The inner loop again is the stochastic sampling loop which assigns probability distributions to uncertain parameters and generates a sample set based on a selected sampling technique (in this case, HSS sampling). The outer loop handles flowsheet synthesis and optimization. This block predicts the decision variables (both discrete

and continuous) and the sample size used by the inner loop. Values of the decision variables and the sample set for uncertain parameters are then transferred to the Aspen model of the superstructure, which configures the flowsheet variant to be analyzed. The probabilistic objective function (e.g., mean, variance, or fractile) and constraints are computed along with the penalty function and transferred to the optimizer. The optimizer then chooses new values of decision variables based on the stochastic annealing algorithm, and the cycle repeats. The termination criteria for the outer optimization loop is governed by either a tolerance imposed on the change in objective function value at the end of each iteration, or the number of temperature levels in the stochastic annealing schedule. Additional details of these procedures are described elsewhere (Chaudhuri and Diwekar, 1996). In practical terms, these new developments provide a capability to handle not only complex process synthesis problems, but also to incorporate uncertainties into the process design stage in a computationally affordable manner.

### APPLICATION TO IGCC DESIGN

Here we turn to an illustration of the new process synthesis capability in the context of a design decision for an IGCC power plant. A typical IGCC system consists of three major sections: gasification, gas cleanup, and power generation. The classification of an IGCC system is based primarily on differences in the gasifier technology, choice of oxidant, and gas cleanup method. Since U.S. coals have a wide range of properties, the choice of coal also can be important, since coal properties can affect the thermal, environmental, and economic performance of IGCC systems.

In the gasification section, coal is gasified in the presence of steam and air or oxygen to produce raw fuel gas. The gasification section typically is followed by a gas cleanup section, where particulates and sulfur compounds are removed along with other contaminants. For advanced IGCC systems, sulfur control is achieved through hot gas cleanup technology using sorbents such as zinc ferrite or zinc titanate. Hybrid systems using a combination of both in-bed and gas stream desulfurization schemes also have been proposed. In addition, cold gas cleanup technologies are used for current commercial systems. Here, fuel gas from the gasifier is cooled to about 100°F so that a low temperature process (e.g., Selexol process) can be used to separate H<sub>2</sub>S from the fuel gas.

After cleanup, the gas stream is combusted in a gas turbine section to generate power. Heat recovered from the turbine outlet stream is used in a heat recovery steam generator (HRSG) for further power extraction via steam turbines. This combined cycle power generation scheme yields higher overall efficiency than the conventional simple cycles used for power generation today.

Different choices of coals, gasifiers, oxidants, emission control systems, and power generation equipment give rise to an array of different system configurations. As the number of options grows, a systematic analysis of all alternative options may be beyond the capabilities or resources of traditional design engineering. For example, a comparison of systems involving six coals, three gasifiers, two oxidants, four gas cleanup methods and two power generation

units would yield a total of 288 different flowsheets that would have to be structured and analyzed individually in Aspen using the current DOE approach. Such an effort would be extremely time-consuming and computationally burdensome. In contrast, the current process synthesis approach would embed all of these design options in the single superstructure representation.

The current study represents a first attempt to synthesize an IGCC flowsheet in the presence of uncertainties. Thus, the problem formulation was kept relatively simple in order to demonstrate the method, and to illustrate the computational efficiency achievable. The case study presented here thus seeks to identify the optimal design configuration based solely on a choice of different coal types and oxidant feeds, involving a total of twelve different options.

### PROCESS DESCRIPTION

The IGCC system modeled in this study (Figure 3) employs the KRW gasifier, which is a pressurized fluidized-bed system operating at 400 psig and 1850°F. Coal is conveyed pneumatically to the base of the gasifier and injected along with the recycle gas and fines. Steam plus oxidant in the form of either air or oxygen react with coal to form a fuel gas stream containing CO, CO<sub>2</sub>, CH<sub>4</sub>, H<sub>2</sub>, H<sub>2</sub>S, COS, and NH<sub>3</sub>. In-bed desulfurization may be performed using limestone or dolomite, which combines with sulfur to form calcium sulfide that is oxidized to calcium sulfate in a sulfation unit. The gas stream leaving the gasifier passes through cyclone filters which remove particulates. The gas then enters a fixed bed zinc ferrite desulfurization section where hydrogen sulfide is selectively adsorbed from the fuel gas by a sorbent consisting of zinc ferrite pellets at 1100°F. The sulfided sorbent is regenerated using air as the oxidant and steam as the diluent, in order to prevent the heat released during the exothermic regeneration reactions from sintering the sorbent. This regeneration off-gas containing SO<sub>2</sub> is then recycled to the gasifier in KRW-based designs (Frey, 1991).

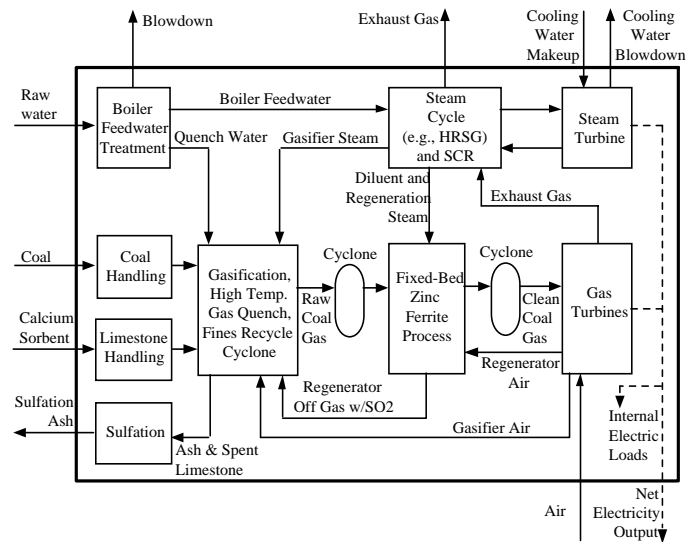


Figure 3. Simplified Schematic of IGCC System (KRW Gasifier with In-Bed and Hot Gas Desulfurization)

The IGCC superstructure, shown in Figure 3, employs both in-bed and gas stream desulfurization. Previous studies based on a deterministic framework showed that this combination of technologies yielded the best economic performance relative to other options (Diwekar and Rubin, 1992b). Therefore, for the purpose of the current synthesis problem, only this option was included in the flowsheet superstructure.

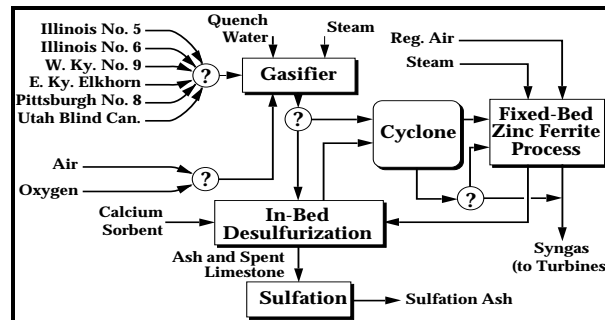


Figure 4. Schematic of Flowsheet Superstructure for IGCC Case Study

The clean fuel gas exiting the zinc ferrite desulfurization section is combusted in a gas turbine operating at 2300°F firing temperature. The combustion products are expanded to 15 psia and 1065°F, subsequently cooled to 262°F in the heat recovery steam generator, then vented through a stack. The HRSG produces steam at 21 psia, 415 psia, and 1480 psia. The low pressure (LP) steam is fed to the deaerator and LP steam turbine. The deaerator supplies feedwater to the intermediate (IP) and the high pressure (HP) boilers. The IP steam is used for NO<sub>x</sub> control in the gas turbine and as gasifier steam. The HP steam is superheated to 985°F and is used to drive the steam turbine.

Significant private and U.S. government resources have been committed to the development of the KRW-IGCC system with in-bed plus gas stream desulfurization. This option therefore defines an important case study for model development and technology evaluation.

### Case Study Assumptions

The IGCC plant modeled is a nominal 700 MW facility operating at an annual capacity factor of 80 percent. Nominal values of process performance and cost parameters, as well as key uncertainties in performance and cost parameters for this system, have been characterized in previous work (Frey et al., 1994). Uncertainty estimates were based on literature reviews, data analysis, and expert judgments of DOE process engineers. Based on this information, probability distributions were developed to quantify the uncertainties in the key input parameters. These uncertainties are shown in Table 1. All input distributions are sampled by the stochastic modeling framework of the Aspen process simulator using the new sampling technique described earlier.

**Table 1. Uncertainty Assumptions for Case Study Plant**

Parameter	Det. Value <sup>a</sup>	Probabilistic Value <sup>b</sup>
<b>PERFORMANCE</b>		
Gasifier temp, °F	1900	T: 1900, 1900, 1950
Carbon Conversion, %	95	T: 90, 95, 97
Oxygen/carbon molar ratio	0.46	T: 0.45, 0.46, 0.47
Fuel NOx conversion, % NH <sub>3</sub> to NO <sub>x</sub>	90	T: 50, 90, 100
Thermal NOx conversion, fraction air N fixated x 10 <sup>5</sup>	4.25	U: 1.0, 7.5
Gasifier NH3 yield, % of coal N	10	T: 0.5, 10, 10
Conversion of CaS to CaSO <sub>4</sub> , %	60	U: 30, 90
Gas turbine CO conversion, wt % CO in fuel gas	98.85	U: 97.72, 99.99
<b>COST PARAMETERS</b>		
Gasifier direct cost uncertainty, % nominal direct capital cost	20	T: 0, 20, 40
Gas turbine direct cost uncertainty, % nominal direct capital cost	25	U: 0, 50
Standard error of HRSG direct cost model, \$ million	0	N:: -17.3, 17.3
Indirect construction cost factor, %	20	T: 15, 20, 25
Project contingency factor, %	17.5	U: 10, 25
Limestone cost, \$/ton	18	T: 18, 18, 25
Ash disposal cost, \$/ton	10	T: 10, 10, 25
Maint. cost factor, gasific., % process area total cost	4.5	T: 3, 4.5, 6
Maint. cost factor, gas turbine, % process area total cost	2	T: 15, 2, 6

<sup>a</sup>Deterministic (nominal) value

<sup>b</sup>T=triangular dist (min, mode, max); U=uniform dist (min,max); N = normal dist (range shown is three standard deviations about the mean)

The principal objectives of this study were to consider the effect of different coal and oxidant choices on the levelized cost of electricity, subject to a sulfur emission constraint, and to select an optimal (least cost) system given the prescribed uncertainties. Six bituminous coals were analyzed (Table 2).

**Table 2. Coal properties for case studies**

Parameter	Ill. No. 5	Ill. No. 6	W. Ky.	E. Ky.	W.VA	Utah
% Ash	7.10	10.00	8.51	5.10	7.30	7.72
% Carbon	77.27	69.53	74.32	77.19	78.60	75.23
% Hydrogen	15.43	5.33	5.12	5.83	5.30	5.37
% Nitrogen	1.88	1.25	1.47	1.35	1.60	1.39
% Chlorine	0.00	0.00	0.04	0.18	0.00	0.01
% Sulfur	1.58	3.86	3.25	1.05	1.70	0.54
% Oxygen	6.74	10.03	7.04	10.24	5.50	9.28
Higher heating value (Btu/lb dry basis)	13,250	12,774	12,245	13,524	13,760	14,140
Unit price (\$/MBtu) as delivered	1.368	1.368	1.601	1.601	1.672	1.341

Mathematically, the optimization problem, based on expected values, can be stated as:

$$\text{Min } C_{\text{elec}}$$

$$\text{s.t. } E_{\text{SO}_2} \leq 0.015 \text{ lbs}/10^6 \text{ Btu}$$

where  $C_{\text{elec}}$  is the expected cost of electricity and  $E_{\text{SO}_2}$  is the sulfur dioxide emission rate. Although this sulfur constraint is far more stringent than current U.S. regulations, it is representative of the capability of advanced IGCC technology, and consistent with DOE's strategic planning objectives (Longwell, et al., 1995).

### Case Study Results

Table 3 summarizes key results from the analysis. The numbers shown are the mean values of the probabilistic result for each case. One sees that the configuration with lowest expected cost of electricity (COE) is the air-blown system using the Utah coal. The most expensive configuration is the oxygen-blown system using Illinois No. 6 coal. Note that the lowest cost system is not the most efficient: the highest thermal efficiency (46.6%) is found to be the air-blown system using the western Kentucky coal. Capital costs also vary across systems, with a mean value range of \$1437 to \$1664 /kW (all costs in constant 1994 dollars). For any particular coal the air-blown system has a lower overall cost than the oxygen-blown system.

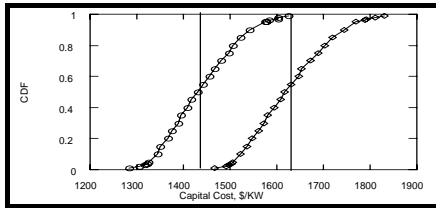
**Table 3. Summary of Case Study Results: Mean Values for Optimal Process Configuration Using Air (Oxygen)**

Parameter	Ill.#5	Ill.#6	W.Ky	E.Ky	W.Va.	Utah
Net Power (MW)	711 (668)	730 (687)	713 (678)	707 (664)	707 (664)	706 (663)
Efficiency (%)	44.3 (40.2)	42.4 (38.9)	46.6 (42.5)	40.5 (36.5)	43.2 (39.0)	42.4 (38.4)
SOx (lb/MBtu)	.0005	.0006	.0007	.0004	.0005	.0004
NOx (lb/MBtu)	0.66 (0.64)	0.49 (0.48)	0.59 (0.57)	0.48 (0.47)	0.57 (0.56)	0.51 (0.50)
Capital Cost (\$/kW)	1452 (1618)	1558 (1664)	1485 (1649)	1448 (1610)	1455 (1626)	1437 (1605)
COE (mills/kWh)	46.3 (50.0)	51.6 (53.3)	49.7 (52.5)	48.2 (51.1)	48.5 (51.6)	45.3 (48.0)

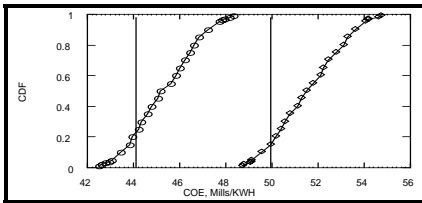
The effect of uncertainties is seen in Figures 5 and 6, which show the cumulative distribution functions (CDF) for the total capital cost and COE, respectively, for the least-cost and highest-cost system configurations. The CDFs in Figure 5 shows an uncertainty of about \$350/kW in the capital cost of each system, with some overlap in the two frequency distributions (i.e., some probability of having the same capital cost). For COE, however, there is no overlap, although an uncertainty is still seen for each technology. These uncertainties reflect the assumptions shown earlier in Table 1.

Since computer optimization methods may sometimes make "knife-edge" choices in meeting an objective function, it is interesting to also examine the difference in cost between the optimum solution, and the next best choice. In this case, the next lowest cost IGCC configuration based on mean COE is the air-blown system using

Illinois No. 5 coal. Figures 7 and 8 show the probabilistic *difference* in



**Figure 5. Total Capital Cost for the Most and Least Expensive Configurations**

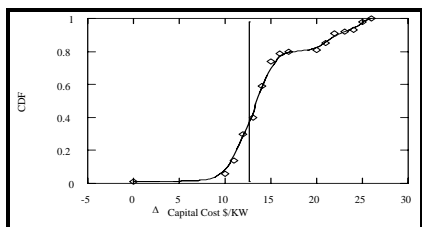


**Figure 6. Total Cost of Electricity for the Most and Least Expensive Configurations**

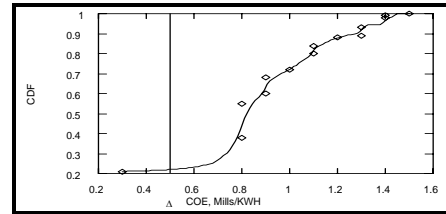
cost between the lowest and second lowest-cost systems. Any uncertain parameters common to the two systems (such as the cost of reagent or ash disposal) are given identical values in each iteration, to insure a systematic comparison. The solid vertical lines in each figure show results from the deterministic analysis.

The CDFs for both the capital cost and COE results show a positive difference over the entire range, indicating that the nominal least-cost configuration is indeed robust over the assumed range of input uncertainties. Note that the CDF is positively skewed relative to the deterministic result, especially for the COE. This indicates the likelihood of a much higher cost savings than predicted from the deterministic analysis. On the other hand, had any of the cost differences been negative, a situation would have been revealed wherein an alternative configuration would have a lower overall cost under some circumstances.

In this particular case study, the stochastic synthesis revealed the same optimal process configuration as a deterministic analysis. The probabilistic analysis, however, showed that this choice is robust in the



**Figure 7. Capital Cost Difference for the Two Lowest Cost Systems**



**Figure 8. Cost of Electricity Difference for the Two Lowest Cost Systems**

face of the technical and economic uncertainties that were specified. In other cases, the inclusion of uncertainties in process synthesis can lead to an altogether different optimum relative to a deterministic analysis (Narayan, et al., 1996). Thus, the new stochastic synthesis capacity demonstrated here can be a powerful tool in identifying designs that are resilient in the face of uncertainties.

### COMPUTATIONAL SAVINGS

To determine the computational efficiency of the stochastic synthesis procedure, a comparative study also was performed in which individual flowsheet simulations for the twelve different coal and oxidant combinations were run for a fixed sample size of 100 samples. Then, the new process synthesis approach was run with all twelve alternative configurations embedded in a single superstructure (Figure 4). A least-cost flowsheet was then synthesized using stochastic annealing.

The single synthesis run yielded the same result as the twelve individual runs. However, stochastic annealing took 36,180 sec of CPU time compared to 89,143 sec for the twelve individual simulation runs. This is a savings of 60 percent, or 15 hours in CPU time alone for this case study. Additional savings accrued in reduced setup time for one large run compared to separate multiple runs. Computational savings are expected to grow as the number of decision variables increases.

### CONCLUSIONS

The large number of technical and economic uncertainties associated with advanced power systems now under development, coupled with an increasingly large array of design alternatives, requires new methods of design and analysis to identify robust, optimal configurations. Individual runs can be computationally intensive as the number of technology options increases, and as uncertainties are included. Stochastic annealing presents an efficient method for screening a large number of alternatives to identify the optimal design configuration in the face of uncertainties.

The case study here applied this new method to identify the optimal combination of coal type and oxidant for an advanced IGCC power generation system now under development. The air-blown variant of the fluidized bed KRW system had a lower expected cost than the oxygen-blown design across a broad range of bituminous coals. The lowest cost combination of coal type and oxidant was found to be a robust choice given the uncertainties considered in the analysis.

The new stochastic synthesis procedure also lowered the computational CPU time by 60% compared to an exhaustive search procedure involving individual flowsheet simulations using the Aspen process simulator. Such relative savings are expected to increase with increasing numbers of flowsheet options. Future work will extend this analysis to include a larger number of flowsheet options for advanced energy systems design.

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