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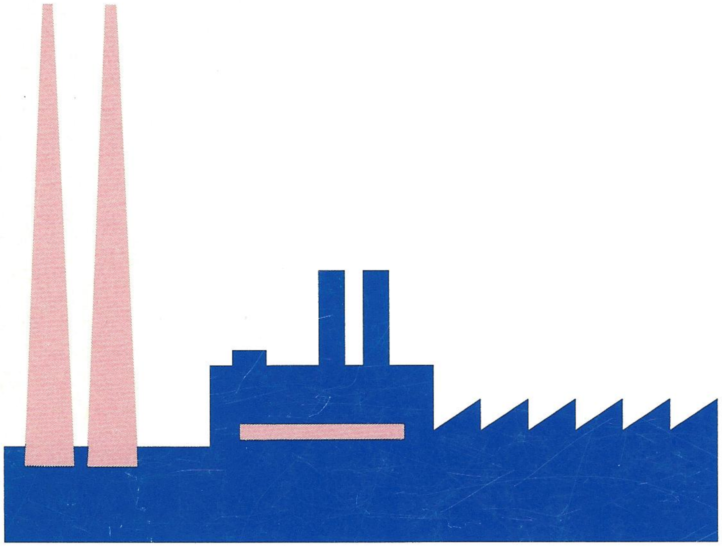

Volume 58 - I

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TECHNOLOGY FOR COMPETITION & GLOBALIZATION

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Proceedings of the

AMERICAN POWER CONFERENCE

Volume 58 - I

Antonia E. McBride, Editor
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ABOUT THE CONFERENCE

The American Power Conference is an annual national forum of ideas concerning aspects of electric power, including: fuels, generation, transmission and distribution. The primary emphasis is on technology as it effects and enables competition and globalization of the power industry. Sponsorship is by the Illinois Institute of Technology (IIT) with the cooperation of professional societies and other universities. The meeting is concurrent and integrated with the annual meeting of the Energy Division of American Society of Civil Engineers. No affiliation is required. Policy is guided by an advisory board.

Presentations at the Conference are by invitation. They are selected from the many abstracts received, following the Call for Papers which is issued in early July preceding the meeting, and due by early September. Invited sessions are organized by experts in certain fields where the subject matter is of particular timely interest. A planning meeting is held at IIT in late September and is attended by members of the Industry-Program Committee. Both regular papers and panel presentations are contributed. Most regular papers and many prepared panel presentations appear in the Proceedings. In some cases, however, circumstances preclude manuscripts being available by the February deadline which is required to permit the Proceedings to be distributed at the meeting. The Table of Contents lists all presentations of record at the time of publication, including late withdrawals and additions. Similar to the Program, presentations are listed by day, AM and PM, and track.

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OPTIMIZATION OF ENVIRONMENTAL CONTROL SYSTEM DESIGN FOR AN IGCC POWER PLANT

URMILA M. DIWEKAR and EDWARD S. RUBIN
Center for Energy and Environmental Studies
Carnegie Mellon University
Pittsburgh, PA 15213 USA

H. CHRISTOPHER FREY
Department of Civil Engineering
North Carolina State University
Raleigh, NC 27695-7908

ABSTRACT

Conventional process models for advanced energy systems are typically based on a deterministic framework in which technical and economic uncertainties are not rigorously treated or characterized. Nor do current design methods rigorously address the issue of process design under uncertainty. Nevertheless, the capability to consider uncertainties in the early stages of advanced power system design is especially important since available performance data typically are scant, accurate predictive models often are unavailable, and many technical as well as economic parameters are not well established. This paper summarizes recent developments in advanced computer-based methods for dealing with uncertainties that are critical to the design of advanced energy systems. Results are presented for an advanced Lurgi-based IGCC system with hot gas cleanup, in which the design of systems for SO_2 removal and NO_x control are optimized to minimize overall costs in the face of performance and cost parameter uncertainties. Risk-based optimization criteria also are explored using stochastic optimization methods.

INTRODUCTION

Environmental regulations have placed new requirements on process design for advanced power systems, and increased the need for more sophisticated simulation and design tools. Conventional process models now in use are typically based on a deterministic framework used to simulate a specified flowsheet. An important shortcoming of these models is their inability to analyze uncertainties. An uncertainty analysis capability is especially important in the context of advanced energy systems, since available performance data typically are scant, accurate predictive models do not exist, and many technical as well as economic parameters are not well established.

Though design under uncertainty has received considerable attention in the literature during the past few years, a generalized framework for analyzing uncertainty systematically has only recently been developed around a chemical process simulator (Ref. 1). In earlier work, we developed a generalized capability to assign probabilistic values to model input parameters, and to sample these distributions to obtain probabilistic results using Latin Hypercube sampling methods. That capability was built around the ASPEN process simulator (Ref. 2) developed for the U.S. Department of Energy (DOE). This stochastic simulation capability has been used successfully to evaluate different configurations of integrated gasification combined cycle (IGCC) systems, an emerging technology for the clean and efficient use of coal for electric power generation. In particular, we have applied probabilistic methods to evaluate the performance, cost, and emissions from IGCC systems, compare alternative systems under conditions of uncertainty, and quantify the benefits from targeted research and development (Refs. 3-5).

More recently, we have enhanced this framework to include a generalized capability to deal with process synthesis (Ref. 6) and process optimization under uncertainty. The new optimization capabilities, built around the public version of ASPEN, are described in this paper. First we describe the methodological basis for these new modeling capabilities, then we present an illustrative case study of their application to the design of environmental controls for an advanced IGCC power system.

METHODOLOGY FOR OPTIMIZATION UNDER UNCERTAINTY

Problems reported in the literature on process design under uncertainty generally are divided into two categories: stochastic optimization, and stochastic programming. Stochastic optimization problems include expected value minimization, chance constrained optimization, and design for optimal flexibility. These problems all require that at each iteration of the optimization solution method some probabilistic representation of the objective function and constraints are optimized. On the other hand, stochastic programming problems involve solving a deterministic optimization problem for each of several "scenarios" to build up a probabilistic representation of optimal solutions. These types of problems show the effects of uncertainties on optimal design. We describe here the new modeling capability developed for these two general categories of optimization problems under uncertainty.

The Optimizer

The goal of a classical optimization problem is to determine the values of decision variables x that maximize some aspect of a deterministic model, represented by the objective function Z, while ensuring that the model operates within limits established by equality constraints h and inequality constraints g. A generalized statement of this problem is given by the following equation

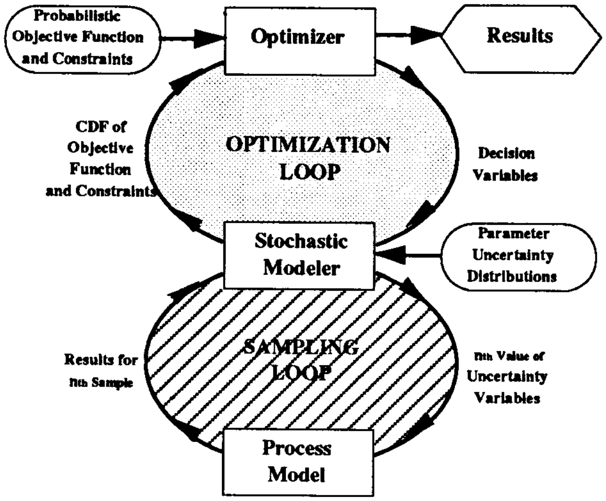

Figure 1. Schematic of the Stochastic Optimization Framework

$$\underset{x}{\text{Optimize}}\ Z = z(x) \qquad (1)$$

$$\text{subject to} \quad h(x) = 0 \qquad (2)$$

$$g(x) \leq 0 \qquad (3)$$

where *x* is a decision variable vector.

A generalized iterative solution procedure for this traditional deterministic optimization problem is employed. The optimizer invokes the model with a set of values for the decision variables *x*. The model simulates the flowsheet and calculates values of the objective function and constraints. This information is utilized by the optimizer to calculate a new set of decision variables. This iterative sequence is continued until the optimization criteria are satisfied. This deterministic optimization capability has been implemented in the public version of ASPEN. A new unit operation block has been developed which solves the nonlinear optimization problem (NLP) described above.

This new NLP optimization capability can be coupled with the stochastic modeling capability developed previously, to solve a broad range of stochastic optimization and stochastic programming problems encountered in practice. The following sections describes this functionality.

Stochastic Optimization

$$\underset{x}{\text{Optimize}}\ P1(Z) = P1(z(x,u)) \qquad (4)$$

$$\text{subject to} \quad P2(h(x,u)) = 0 \qquad (5)$$

$$P3(g(x,u) \leq 0 \qquad (6)$$

where *u* is the vector of uncertain parameters and the *P* represents the probabilistic functional. For problems where the goal is to minimize an expected value this reduces to:

$$E(F(u)) = \int_0^1 F(u)dp(u) \qquad (7)$$

This function can be calculated by sampling the function and calculating the expected value of the samples.

$$E(F(u)) = \frac{\sum_1^{N_{samp}} F(u)}{N_{samp}} \qquad (8)$$

On the other hand, for chance constrained optimization problems, where the constraints are represented in terms of a probability of exceeding a certain value, the probabilistic functional is represented by:

$$\underset{x}{\text{Optimize}}\ P1(z(x,u)) = E(F(u)) \qquad (9)$$

$$\text{subject to} \quad P(h(x,u) > \beta) \leq P_C \qquad (10)$$

where Equation 10 is a chance constraint.

Unlike the deterministic optimization problem, in stochastic optimization one has to consider the probabilistic functional of the objective function and constraints. The generalized treatment of such problems is to use probabilistic or stochastic models instead of a deterministic model inside the optimization loop. Figure 1 represents the generalized stochastic optimization problem solution procedure, where the deterministic model is replaced by an iterative stochastic model.

Stochastic Programming

In contrast to the stochastic optimization problems, stochastic programming problems concern the effect of uncertainties on optimal design. This involves deterministic decisions at each random stage or random sample, which is the same as solving multiple deterministic optimization problems. This formulation can be represented as:

$$\underset{x}{\text{Optimize}}\ Z = z(x,u^*) \qquad (11)$$

$$\text{subject to} \quad h(x,u^*) = 0 \qquad (12)$$

$$g(x,u^*) \leq 0 \qquad (13)$$

where *u** is the vector of values of uncertain variables corresponding to a particular sample. This optimization procedure is repeated for each sample of uncertain variables *u* and a probabilistic representation of outcomes is obtained. Figure 2 represents the generalized solution procedure, where the deterministic problem shown in Figure 1 forms the inner loop and the stochastic sampling forms the outer

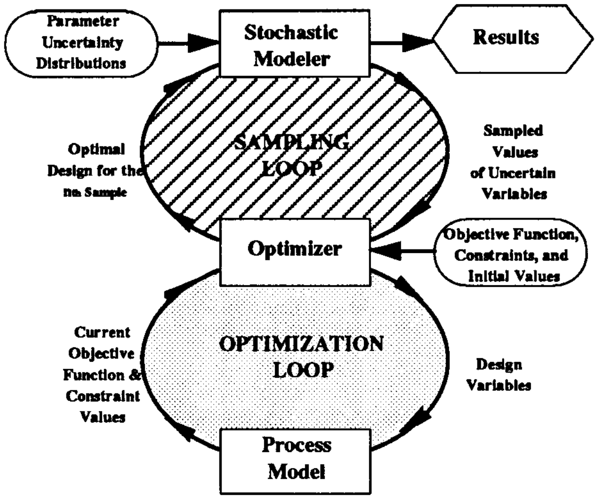

Figure 2. Schematic of the Stochastic Programming Framework

loop. This procedure is implemented in the ASPEN simulator by simply interchanging the position of stochastic block, and the optimization block. In this way, one can solve almost all the problems in the stochastic optimization/programming literature.

APPLICATIONS OF THE NEW MODELING CAPABILITIES

The new capabilities for process synthesis and optimization under uncertainty provide powerful new tools for the design and analysis of advanced energy systems. In this paper we illustrate the use of the stochastic optimization and stochastic programming capabilities for the design and analysis of advanced IGCC systems now under development.

IGCC Process Description

Conventional IGCC designs are based on "cold" gas cleanup, in which the fuel gas from the gasifier is cooled to a sufficiently low temperature (e.g., 100°F) that a commercial sulfur removal process can be used to separate H_2S from the fuel gas. A focus of current research is the development of "hot" gas cleanup systems, in which sulfur compounds may be removed from the gasifier or the fuel gas at high temperature (e.g., 1000°F). Hot gas cleanup eliminates the capital cost associated with heat exchangers needed to cool the fuel gas, and treatment systems needed to handle process condensates resulting from fuel gas cooling. Hot gas cleanup also reduces the thermal efficiency penalty associated with gas cooling, allowing the sensible heat of the high temperature fuel gas to be supplied directly to the gas turbine.

One hot gas cleanup configuration that has been under investigation is an air-blown Lurgi gasifier-based IGCC system. The higher cold gas efficiency of Lurgi gasifiers compared to other gasifiers can result in a higher plant efficiency, because a larger portion of the energy input enters the combined cycle system through the fuel gas rather than only through the steam cycle. The conversion efficiency of energy entering the gas turbine is much higher than that of energy entering the steam cycle. The exit temperature of syngas from a Lurgi or similar gasifier also provides a more direct match with the temperature window of hot gas cleanup systems, thereby eliminating any requirement for syngas cooling. Lurgi-based IGCC systems with hot gas cleanup therefore offer the potential for simplified plant designs (Ref. 7).

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

Other hot gas cleanup systems for Lurgi-based IGCC plants also are being developed. General Electric is testing a moving-bed zinc titanate desulfurization system in which sorbent circulates continuously between an absorber and regenerator vessel (Ref. 8). The moving bed design offers advantages in terms of a steady flow of regeneration off-gases and the elimination of steam requirements as a diluent. However, at this time only limited design data and no detailed cost data are publicly available for this proprietary system.

Case Study Design

A 650 MW IGCC system featuring an air-blown dry ash Lurgi gasifier using a high-sulfur Illinois No. 6 coal is analyzed in this paper. A hot gas cleanup system is used for high temperature (600°C) sulfur removal using the zinc ferrite system, with high efficiency cyclones and ceramic filters for particulate removal. Details of the performance and cost models for this system are reported elsewhere (Ref. 3).

Two key design variables for the fixed bed zinc ferrite process are the sulfur absorption cycle time and the reactor vessel length-to-diameter ratio. The sulfur absorption cycle time is constrained to be at least as great as the time required to regenerate a bed of sulfated sorbent and return it to active service after a regeneration cycle. As the sulfur absorption time becomes longer, more sorbent is required to capture the syngas sulfur species over the increased time period. Larger absorption cycle times therefore require either larger reactor vessels and/or more reactor vessels, which increases the cost. The length-to-diameter ratio of the reactor vessel also affects process economics.

Another key area of uncertainty for this technology is the NO_x emission rate. Thermal NO_x emissions are expected to be quite low for IGCC systems due to the low heating value of the fuel gas and the presence of thermal diluents such as H_2O, CO_2, and N_2 (Ref. 9). However, the hot gas cleanup system employed by the air-blown Lurgi system does not remove fuel-bound nitrogen (in the form of ammonia) from the fuel gas, and a substantial portion of the ammonia is converted to NO_x upon combustion. Thus, NO_x emissions pose a critical concern for systems with hot gas cleanup. For example, using conventional combustors the DOE performance model of the Lurgi-based IGCC system yields NO_x emissions nearly four times greater than U.S. federal New Source Performance Standard (NSPS) of 260 ng/J (0.6 lbs/10^6Btu) for coal-fired power plants. Future levels of NO_x emissions are likely to be subject to much more stringent requirements because of the role of NO_x in acid rain and tropospheric ozone formation.

To mitigate NO_x emissions, several approaches are possible. In the near term, the most likely approach is the use of post-combustion exhaust gas NO_x reduction technology. In the longer term, advanced staged combustion designs featuring rich/lean combustion may be commercialized and employed for fuels with high nitrogen content.

In this study, we consider the use of selective catalytic reduction (SCR) for NO_x control. In a SCR system, ammonia is injected into the flue gas upstream of a catalytic reactor through a set of nozzles comprising an injection grid. Because of the temperature window required for typical SCR catalysts, the SCR reactor employed with gas turbine combined cycle systems is typically located in the heat recovery steam generator. We employ a new performance and cost model of an SCR system (Ref. 10) to explore the effects of two key design variables: the required NO_x removal efficiency, which has a substantial impact on the catalyst volume requirement, and the catalyst layer replacement interval, which can be varied to achieve trade-offs between initial capital cost and annual replacement costs for catalyst. Since the cost of catalyst is a major expense for SCR systems, optimizing this process design is of significant interest.

Uncertainty Assumptions

Key performance and cost parameters of the engineering models for the IGCC system were assigned probability distributions based on data analysis, literature review, and the elicitation of expert judgments. The characterization of performance uncertainties focused on four major process areas: gasification, zinc ferrite desulfurization, gas turbine, and the SCR unit. Uncertainties in additional cost model parameters also were characterized, including direct and indirect capital costs, operating and maintenance costs, financial assumptions, and the unit costs of consumables, byproducts, and wastes. Through an interactive screening process, the initial set of approximately 50 uncertain variables was narrowed to a set of 20 which most significantly affected uncertainty in plant efficiency, emissions, capital cost, and total levelized cost. These variables are listed in Table 1.

Results of Optimization Studies

Figures 3 to 5 show the results of different stochastic optimization and stochastic programming problems applied to the IGCC flowsheet. Figure 3 first shows results of a stochastic optimization problem in which the expected cost of electricity (COE) is minimized for different levels of NO_x control (note that mills/kWh is identical to dollars/MWh). As the expected (mean) value of NO_x emissions is decreased, the expected value of NO_x removal efficiency in the SCR unit increases proportionally. The cost of the optimal design also increases linearly. As seen in Figure 3, the optimal design reduces the expected COE by 0.5 mills/kWh relative to the base case design achieving 0.44 lbs NO_x /10^6 Btu. For the 650 MW plant modeled in this example, this is equivalent to a total savings of approximately $2 million per year. This savings is a measure of the benefit resulting from use of the new stochastic method to optimize the design parameters of the zinc ferrite and SCR units. Figure 3 also shows that the expected cost of the optimal design increases by 0.6 mills/kWh as NO_x is lowered from 0.6 to 0.22 lbs/10^6 Btu. This provides an indication of the expected cost impact of a threefold tightening of current U.S. standards. Over this range, the optimal SCR removal efficiency increases from 73% to 90%, the latter being the maximum value established by the performance model.

To illustrate results for a stochastic programming

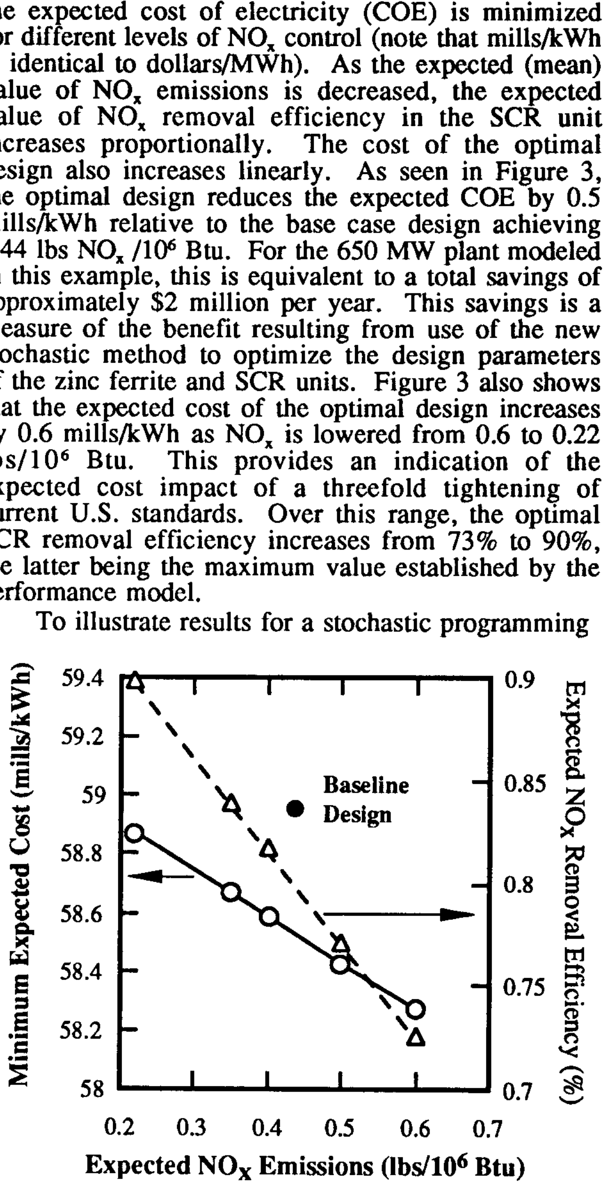

Figure 3. Minimization of Total Levelized Cost Subject to Executed Value of NO_X Emission Constraint

Table 1. Uncertain Model Parameters for Illustrative Case Studies

DESCRIPTION AND UNITS (a)	Val (b)	Type	Min	Max	Prob.
Gasifier Fines Carryover, wt-% of Coal Feed	5.0	F	0.0	1.0	5%
			1.0	3.5	20%
			3.5	5.0	25%
			5.0	8.0	25%
			8.0	15.0	15%
			15.0	20.0	5%
			20.0	30.0	5%
Fines Capture in Recycle Cyclone, wt-% of Fines Carryover	95	F	50	90	25%
			90	95	25%
			95	97	25%
			97	98	25%
Carbon Retention in the Bottom Ash, wt-%	2.5	T	0.75	10.0	2.5
Gasifier Coal Throughout, lb DAF coal/(h-ft2)	305	T	1.52	381	305
Gasifier NH3 Yield, % of coal-N converted	0.9	T	0.5	1.0	0.9
Gasifier Air/Coal Ratio, lb air/lb DAF coal	3.1	T	2.7	3.4	3.1
Steam/Coal Ratio, lb steam/lb DAF coal					
air/coal = 2.7	0.81	U	0.54	1.08	
air/coal = 3.1	1.55	U	1.24	1.86	
air/coal = 3.4	2.38	U	2.04	2.72	
Zinc Ferrite Sorbent Sulfur Loading, wt-% sulfur in sorbent	17.0	N	2.16	31.84	17.0
Zinc Ferrite Sorbent Attrition Rate, wt-% sorbent loss per absorption cycle	1.0	F	0.17	0.34	5%
			0.34	0.50	20%
			0.50	1.10	25%
			1.10	1.50	25%
			1.50	5.00	20%
			5.00	25.00	5%
Fuel NOx, % conversion of NH3 to NOx	90	T	50	100	90
Gasifier Direct Cost Uncertainty, % of estimated direct capital cost	20	U	10	30	
Sulfuric Acid Direct Cost Uncertainty, % of estimated direct capital cost	10	U	0	20	
Gas Turbine Direct Cost Uncertainty, % of estimated direct capital cost	25	U	0	50	
SCR Unit Catalyst Cost, $/ft3	840	U	250	840	
Standard Error of HRSG Direct Cost Model, $Million	0	N	-17.3	17.3	
Maintenance Cost Factor, Gasification, % of process area total cost	3	T	2	12	3
Maintenance Cost Factor, Combined Cycle, % of process area total cost	2	T	1.5	6	2
Unit Cost of IC Ferrite Sorbent, $/lb	3.00	T	0.75	5.00	3.00
Indirect Construction Cost Factor, %	20	T	15	25	20
Project Contingency Factor, %	17.5	U	10	25	

(a) DAF = dry, ash free; SCR = selective catalytic reduction; HRSG = heat recovery steam generator (b) DET. VAL. = deterministic (point-estimate) value. The next column indicates the type of distribution, where F = fractile, T = triangular, N = normal, and U = uniform. The remaining columns provide the parameters of the distribution.

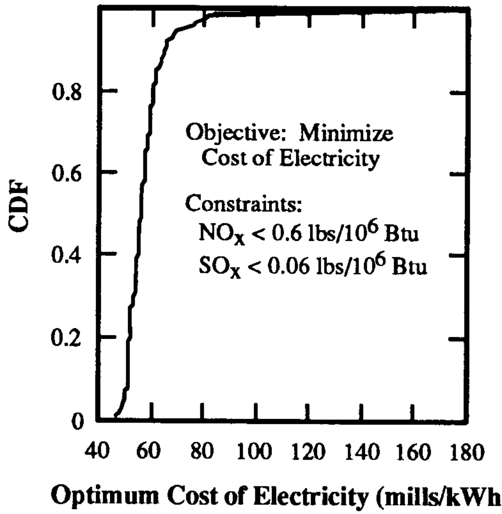

Figure 4. Effect of Uncertainties on Minimum Cost of the Lurgi IGCC System

formulation, Figure 4 next shows the effect of uncertainties on the cost of an optimal design. Here, for each sample the cost is minimized and NO_x emissions are constrained to 0.6 lbs/10^6 Btu or less, and SO_2 emissions 0.06 lbs/10^6 Btu or less (the DOE design goal of one tenth the current U.S. federal standard). The cost of electricity for the optimal design configuration is seen to vary by more than a factor of four due to the performance and cost uncertainties in the variables shown in Table 1. An 80% confidence interval gives expected costs between 45.0 and 60.0 mills/kWh.

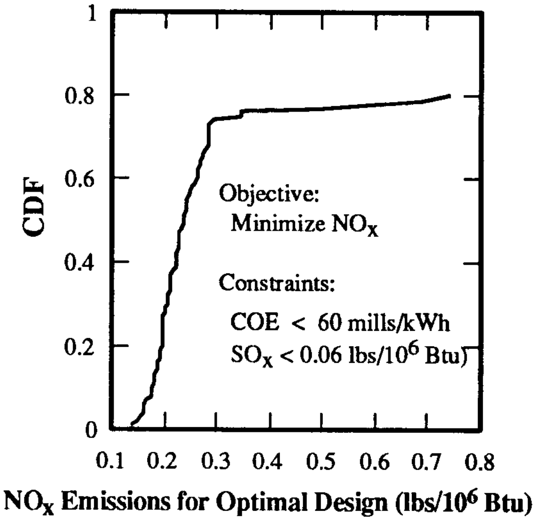

Figure 5. Effect of Uncertainties on Minimum NO_X Emissions For a Given Cost Constraint

Figure 5 shows another example in which NO_x emissions are minimized subject to a cost constraint. There is a 20% probability that the cost will exceed 60 mills/kWh. For the remaining 80% of the optimal designs which are within the cost constraint, 2% of these designs will exceed 0.6 lbs/10^6 Btu of NO_x, the Federal New Source Performance Standard for coal-fired power plants. For these cases, there is a significant risk that the process may not be viable under the economic constraints imposed in this example, since the plant might not comply with applicable emission limits.

CONCLUSIONS

This paper has described a set of new systems analysis tools and methods that can substantially improve the design and analysis of advanced coal-based energy systems. By enhancing existing process simulators with the mathematical methods presented here, researchers and research managers now can tackle a wide range of system performance and cost analysis not heretofore possible. This new toolbox can be used in conjunction with new or existing process performance and cost models to insure that process design issues are more fully and rigorously considered in all phases of activity. These modeling tools also can be extended to a host of other technology applications where process design, cost minimization, risk analysis, environmental compliance, and R&D prioritization remain important issue.

Additional case studies for other advanced power systems, including other IGCC designs, pressurized fluid bed combustion (PFBC) systems, and externally fired combined cycle (EFCC) systems also are in progress. In conjunction with these efforts, on-going work also is developing new or improved cost and performance models for selected process components and systems for IGCC, PFBC and EFCC designs. These new models can form the basis for systematic comparisons of alternative coal-based power systems, and the effects of uncertainties on their optimal design, cost and performance

ACKNOWLEDGEMENTS

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CATALYTIC REBURNING FOR NO_x CONTROL IN ADVANCED COAL-BASED POWER GENERATION

ARDEN B. WALTERS
President
Advanced Energy Research, Inc.
Delray Beach, Florida

M. A. VANNICE
Professor
XIANKUAN ZHANG
Post-Doctoral Fellow
SHU-JIUAN HUANG
Ph.D.Graduate Student
Department of Chemical Engineering
The Pennsylvania State University
University Park, Pennsylvania

INTRODUCTION

This paper describes a new NO_X decomposition and selective reduction catalyst system that uses fuel gases, rather than a reagent, such as ammonia, as the reductant. These catalysts are expected to have many applications for new advanced coal-based power generation and for advanced technology retrofits and upgrades of existing power plants.

Advanced coal-based technologies for power generation include technologies for new power plants and technologies for power plant retrofits, for technologies using coal directly and for technologies using coal-based synfuels. These advanced coal-based power generation technologies typically share in common the need for NO_X emission control, but significant differences in these technologies require the tailoring of NO_X reduction approaches to achieve the most effective NO_X control for each.

Some advanced coal-based power generation technologies, e.g., coal-synfuel-based fuel cells, should generate very little NO_X, and others, e.g. fluidized-bed boilers, are inherently capable of significantly reducing thermal NO_X formation (although added NO_X reduction technologies, such as ammonia SNCR are sometimes required). And, special burners or other adjustments in combustion conditions for boilers, gas turbines, and other engines that use coal directly, or use coal-based synfuels, can also greatly reduce NO_X formation. But, even with technologies for the minimization of NO_X formation, there remains a need for post-combustion NO_X control (PCNOX).

Much of the need for PCNOX comes from increasingly stringent regulations. These regulations can even require that PCNOX be added downstream of other technologies that reduce NO_X formation. This could be especially true for coals and coal-based synfuels with high nitrogen contents and for existing coal-fueled power plants not well-suited for advanced coal-based technologies, such as special burners and other adjustments to combustion conditions, e.g. EPA Group 2 boilers (cyclone, wet bottom wall-fired, cell burner, stoker, and some other coal-fired boiler types). And, in addition to the existing coal-based power generation units that might require PCNOX for retrofits, there are also new, advanced coal-based power generation technologies and applications that will require PCNOX.

Post-Combustion NO_X Control

Despite the many advances in the use of modified fuel-air mixing and combustion catalysts in low-NO_X burners, PCNOX is still needed for many NO_X sources. PCNOX includes three major approaches to the control of NO_X emissions. These are NO_X decomposition,

$$2NO_X \rightarrow N_2 + xO_2 \qquad (1)$$

NO_X reduction,

$$2NO_X + (\text{reductant}) \rightarrow N_2 + (H_2O, CO_2, \text{other}) \qquad (2)$$

and NO_X collection,

$$NO_X + (\text{absorbent/adsorbent}) \rightarrow (\text{used sorbent}) \qquad (3)$$

Some PCNOX technologies will involve a combination of these three major approaches to NO_X control. And, unlike NO_X decomposition and reduction, NO_X collection will require either spent sorbent disposal or regeneration; regeneration will require additional processing to decompose, reduce, or re-collect NO_X or other NO_X-derived material.

For typical conditions in coal-based power generation flue gases NO_X decomposition is possible only with the assistance of catalysts. NO_X reduction and NO_X collection can be accomplished with or without the assistance of catalysts.

Post-combustion NO_X reduction for low excess air NO_X sources is achieved by catalytic and non-catalytic processes that use either typical fuels (including partially burned intermediates) or fixed-nitrogen reagents (primarily ammonia) as reductants. NO_X reduction for high excess air NO_X sources requires the use of a selective catalyst and a special reducing reagent, such as ammonia.

The *non-catalytic reburn* process for NO_X reduction injects hydrocarbon fuels, typically natural gas, to create a slightly fuel-rich, high-temperature, post-combustion zone where NO_X is reduced by free radicals. This homogeneous reaction zone is followed by a burn-out zone where enough