Paper Number:
DOE/MC/29094-97/C0713

Title:
Optimizing Advanced Power System Designs Under Uncertainty

Authors:
E.S. Rubin
U.M. Diwekar
H.C. Frey

Contractor:
Carnegie Mellon University
Baker Hall 128-A
Pittsburgh, PA 15213

Contract Number:
DE-AC21-92MC29094

Conference:
Advanced Coal-Fired Power Systems '96 Review Meeting

Conference Location:
Morgantown, West Virginia

Conference Dates:
July 16-18, 1996

Conference Sponsor:
U.S. DOE, Morgantown Energy Technology Center

Disclaimer

OPTIMIZING ADVANCED POWER SYSTEM DESIGNS UNDER UNCERTAINTY

E.S. Rubin and U.M. Diwekar
Carnegie Mellon University
Pittsburgh, PA 15213

H.C. Frey
North Carolina State University
Raleigh, NC

ABSTRACT
This paper describes recent developments in ongoing research to develop and demonstrate advanced computer -based methods for dealing with uncertainties that are critical to the design of advanced coal-based power systems. Recent developments include new deterministic and stochastic methods for simulation, optimization, and synthesis of advanced process designs. Results are presented illustrating the use of these new modeling tools for the design and analysis of several advanced systems of current interest to the U.S. Department of Energy, including the technologies of integrated gasification combined cycle (IGCC), advanced pressurized fluid combustion (PFBC), and the externally fired combined cycle (EFCC) process. The new methods developed in this research can be applied generally to any chemical or energy conversion process to reduce the technological risks associated with uncertainties in process performance and cost.

INTRODUCTION
Increasing environmental awareness and regulations have placed new requirements on process design for advanced power systems, and increased the need for more sophisticated simulation and design tools to examine pollution prevention options. Conventional process models now in use are largely based on a deterministic framework for simulation of a specified flowsheet. An important shortcoming of these models is their inability to analyze uncertainties rigorously. 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.

In essence, the current project is focused on developing better ways to minimize technological risk by seeking process designs that minimize the likelihood of performance shortfalls, high emissions and high costs. A related goal is to help focus research and development in areas that offer the greatest potential payoffs in terms of process efficiency, emissions and cost. Our thesis is that advanced design and analysis methods are needed in light of the increasing complexity of advanced processes, involving multiple options for component design and selection; strong interactions among system components (which often can be overlooked by traditional design methods); and significant performance and cost uncertainties, particularly for processes at an early stage of development.

The approach adopted in this research has been one that employs a systems analysis framework that combines engineering models of process performance with companion models of process costs, and which utilizes advanced software capabilities for design and analysis. In this project, we have specifically focused on advanced technologies of interest to the U.S. Department of Energy's Morgantown Energy Technology Center (DOE/METC). Thus, the technologies modeled and evaluated in this research include various types of integrated coal gasification combined cycle (IGCC) system, including both air-blown and oxygen blown gasifiers; fixed-bed and fluidized bed gasifiers; hot gas and cold gas clean up systems; and a variety of by-product recovery options, including sulfur and sulfuric acid recovery by conventional (e.g., Claus plant) and advanced (e.g., direct sulfur reduction process) methods. Other advanced systems analyzed include advanced pressurized fluidized bed combustion (PFBC) systems and externally fired combined cycle (EFCC) systems.

In all of these areas, we have utilized existing DOE/METC computer models of process thermal performance, and have enhanced these models in a number of areas, including the characterization of emissions, and the coupling of process performance and economics via models of capital cost, operating costs, and overall cost of electricity. Details of these models are summarized in a series of topical reports dealing with specific technologies (CMU, 1990; 1995).

In this project, we also have developed a set of new analytical modeling capabilities built around the public version of the Aspen process simulator used by DOE/METC for advanced process modeling. These new capabilities include both deterministic and stochastic methods for process simulation, process optimization, and process synthesis. The stochastic methods, which explicitly incorporate uncertainties into the design and analysis stage, represent an especially important capability which has not heretofore been available. The remainder of this paper briefly describes these new modeling tools and their applications to advanced coal-based technologies.

SIMULATION CAPABILITIES

Conventional process modeling involves deterministic simulation in which parameter values are input to a process model, yielding results for the quantities of interest (e.g., thermal efficiency, emissions, cost). In many cases, the process models used for deterministic simulations may be quite detailed, as is the case with several of the Aspen models developed by DOE for advanced energy conversion processes. Nonetheless, a characteristic of deterministic models is that each of the input parameters specified for given model run has only a single value, and similarly all of the results are single-valued.

However, many model parameters may in fact have significant uncertainty or variability that can lead to significant uncertainties in the results, particularly for processes at an early stage of development. In stochastic simulation, these uncertainties are incorporated explicitly. Input parameters are described as uncertainty distributions which are sampled by the stochastic modeling software and developed for the Aspen simulator (Diwekar and Rubin, 1991). The results can then be displayed as a cumulative distribution function showing the likelihood of different outcomes for a given simulation. Information on input uncertainties may come from a variety of sources, including data analysis and expert judgments. Previous papers and reports have elaborated on this methodology, and displayed results from case studies of IGCC systems which often showed significant probability of performance shortfalls and cost overruns relative to nominal or deterministic analyses (Frey and Rubin, 1992a).

In our more recent work, we have extended stochastic simulations to include two new process flowsheets, the EFCC system and the second generation PFBC system. Figure 1 illustrates one result from an analysis of the EFCC plant efficiency. Though this technology is expected to achieve net thermal efficiencies significantly higher than those of conventional pulverized coal power plants, the magnitude of efficiency revealed by the probabilistic analysis is generally lower than the result from conventional deterministic simulation. In this case, the performance shortfall is attributed primarily to uncertainties in the process combustor and ceramic heat exchanger, which were characterized by experts at DOE/METC. Figure 1 indicates over a 95 percent probability of a performance shortfall.

In Figure 2, results are presented for the total capital cost of a second generation PFBC system. This technology appears to have a lower cost than most of the IGCC systems previously analyzed. However, a stochastic simulation indicates a very high probability that the total capital cost will exceed the deterministic estimate developed for DOE in a detailed 1989 study. In this case, the potential for higher cost is attributed primarily to uncertainties in various indirect cost factors, particularly the process and project contingency costs.

In previous papers (Frey and Rubin, 1992a; 1992b; Frey et al., 1994), we have shown how stochastic simulation methods can help identify and reduce technological risks such as costs overruns and performance shortfalls by identifying the factors that contribute most to overall uncertainty, and targeting R&D in these critical areas. Quantitative measures of the value of additional research can be developed in conjunction with these methods.

OPTIMIZATION CAPABILITIES

In the current research project we have extended the set of modeling capabilities to include both deterministic and stochastic optimization of process flowsheets. Deterministic optimization is well established in the technical literature, and some commercial simulators have such capabilities. The problem typically is formulated in terms of an objective function to be achieved (e.g., cost minimization) subject to specified constraints. The optimizations software begins with a set of initial values for process parameters and iterates until the objective function is achieved. Details of this problem formulation are presented elsewhere (Diwekar et al., 1993).

We have added a deterministic optimization capability to the public version of the Aspen simulator, and also have combined this feature with the stochastic sampling capability described earlier, yielding new capabilities for stochastic optimization and stochastic programming. In stochastic optimization, depicted in Figure 3, the objective function can be specified probabilistically, as can the constraints. An objective function might be specified in terms of minimizing an expected value, or use chance constraints to minimize a given technological risk (e.g., no more than a 5 percent chance of a performance shortfall). By inverting the sampling and optimization loops, various stochastic programming problems also can be addressed. Such problem formulations reveal the effects of uncertainty on optimal designs. The mathematical formulation of stochastic optimization and programming problems is described in Diwekar et al., 1993.

These new capabilities allow a broad range of questions to be addressed. For example:

- Is there a better choice of parameter values for this process to improve its performance? To lower its cost?
- What levels of performance and cost can we expect from an optimized design?
- How do uncertainties in process performance and cost variables affect the optimal design?
- What design choices will minimize the risk of a performance shortfall? Or the risk of a cost overrun?

Applications

We illustrate the new optimization capabilities with a case study of the environmental control system design for an advanced IGCC system employing hot gas cleanup (HGCU). Systems with HGCU promise higher thermal efficiency than conventional systems with cold gas cleanup. However, one potential drawback is that NO_x emissions can be high because ammonia in the fuel gas is not removed by the HGCU unit, and thus can be converted to NO_x in the combustor. For current process design, this may result in NO_x emissions that are two to four times higher than the Federal New Source Performance Standard for coal-fired power plants. NO_x control methods employing advanced stage combustion are currently under development in an attempt to address this problem. In this case study, we examine the use of selective catalytic reduction (SCR) systems to reduce NO_x emissions. A detailed model of an SCR process has been developed (CMU, 1995) and incorporated into the Aspen flowsheet for a 650 MW IGCC system employing an air-blown moving bed gasifier. The plant uses an Illinois No. 6 coal and operates at an annual capacity factor of 80 percent. Uncertainties have been assigned to 20 key parameters identified in screening studies as having the greatest impact on process performance, emissions and costs. Table 1 summarizes these input assumptions.

Figures 4 to 6 show the results of different stochastic optimization and stochastic programming problems applied to the IGCC flowsheet. Figure 4 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. 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 expected cost of the optimal design also increases, as seen in Figure 4. A key finding is that the optimal design reduces the expected COE by about 0.3 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 5 shows another example in which NO_x emissions are minimized subject to a cost constraint. For a cost constraint of 60 mills/kWh, emissions between 0.15 and 0.3 lbs/10^6 Btu can be achieved. However, for a tighter constraint of 54 mills/kWh, only 80% of the optimal designs are within the cost constraint, and some 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.

To illustrate results for a stochastic programming formulation, Figure 6 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 and 60 mills/kWh.

These results are intended only to be illustrative of the new modeling capabilities now possible with stochastic optimization and stochastic programming. 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 will be the subject of other reports.

SYNTHESIS CAPABILITY

In process simulation and optimization, the flowsheet being analyzed already has been specified by a knowledgeable process designer. In process synthesis, we employ computer-aided design tools to ask what the flowsheet should look like in the first place in order to achieve process goals and reduce technological risks.

We have previously described the formulation of a deterministic process synthesis problem involving mixed integer non-linear programming (MINLP) (Diwekar et al., 1991). This capability now has been implemented around the public version of the Aspen simulator, yielding a new capability that does not currently exist in most commercial simulators.

Figure 7 shows this capability schematically. The synthesis loop begins with a superstructure of all possible alternatives for combining unit operations into a process flowsheet. The mixed integer linear programming (MILP) master program selects a given flowsheet topology, which is then passed to the non-linear programming (NLP) optimization loop described earlier. The optimizer then selects values of continuous variables to meet specified objective functions and constraints. The overall process is then repeated in the synthesis loop until a flowsheet topology and design parameter that best meets desired objectives are found.

An initial case study to demonstrate this capability involved choosing a desulfurization system to minimize the total cost of an IGCC system employing an air-blown KRW gasifier with hot gas cleanup, subject to an SO_2 emission constraint of less than 0.015 lbs/million Btu. In this case, there were three possible flowsheet options: in-bed sulfur removal only; gastream cleanup only; and combined in-bed plus gas stream cleanup. Each option yielded a different waste or byproduct stream which also was considered in the design.

Details of this case study are reported in Diwekar et al., 1992. The MINLP selected the combination of in-bed plus gas stream desulfurization as the optimal configuration, and optimized the design parameters of the zinc ferrite desulfurization system to achieve minimum cost. The total cost of the optimized configuration was approximately 20 percent less than the next best alternative, illustrating the power of this new analytical method.

Recently, we have extended the process synthesis capability to include more complex design alternatives, such as the synthesis problem depicted in Figure 8. Because the MINLP approach is not well suited to some types of synthesis problems, we have applied the method of simulated annealing to handle complex problems more efficiently. We also have developed a new variant of simulating annealing, called stochastic annealing, which offers far greater computational speed, and is well suited to handling problems of process synthesis under uncertainty. For example, for the twelve design choices represented in Figure 8 by the choice of coals and air or oxygen-blown gasification, the stochastic synthesis problem was solved in nearly one fifth the time required to solve the twelve problems individually. These new methods thus appear to offer substantial benefits in addressing complex design problems that have heretofore not been amenable to computer-aided approaches.

CONCLUSIONS

The key message stemming from the work described in this paper is that we now have a power new set of computer-based design tools that can be generally applied to any chemical or energy conversion process. These tools include both deterministic and stochastic capabilities for process simulation, process optimization, and process synthesis. Applications of these new tools can help minimize technological risks and maximize research productivity by considering uncertainties in the early stage of design and analysis.

Future work will continue to focus on methodological improvements to enhance the speed and versatility of the new analytical techniques described in this paper. At the same time, new case studies will be undertaken to enhance process flowsheets and demonstrate the power and applicability of advanced analysis methods to real engineering and process design problems of interest to DOE and its contractors. Key areas for application of these models will include process design, risk analysis, cost estimation, R&D management, technology evaluation, environmental compliance, marketing studies, and strategic planning.

ACKNOWLEDGEMENTS
The authors happily acknowledge the important contributions to this project made by graduate students Prosenjit Chaudhuri and Donna Riley at Carnegie Mellon University, and Pankaj Agarwal at North Carolina State University. This work was supported under Contract No. DE-AC21-92MC29094

REFERENCES

Diwekar U. M. and E. S. Rubin, 1991, Stochastic Modeling of Chemical Processes, *Comput. Chem. Engng.*, **15**, 105.

Diwekar U. M., I. E. Grossmann, and E. S. Rubin, 1991, An MINLP process synthesizer for a sequential modular simulator, *I&EC Res.*, **31**, 313.

Diwekar U. M., H. C. Frey, and E. S. Rubin, 1992, Synthesizing optimal flowsheets: applications to IGCC system environmental control, *I&EC Res.*, **31**, 1927.

Diwekar U. M., E. S. Rubin and H.C. Frey, Optimization of Advanced Energy Systems Under Uncertainty, *Proceedings of METC Contractors Meeting*, U.S. Department of Energy, Morgantown, WV.

CMU 1990, "Stochastic Modeling of Coal Gasification Combined Cycle Systems: Cost Models for Selected Integrated Gasification Combined Cycle (IGCC) Systems," Task 2 Topical Report, Morgantown Energy Technology Center, Morgantown, WV.

CMU, 1995, Development and Application of Optimal Design Capability for Coal Gasification Systems, Task 1 Topical Report, Volumes 1-4: Vol. 1: "Development and Application of Performance and Cost Models for Gas Turbine Based Selective Catalytic Reduction NOx Control." Vol. 2: Development and Application of Performance and Cost Models for The Externally Fired Combined Cycle." Vol. 3: "Performance and Cost Models for the Direct Sulfur Recovery Process," Vol. 4: "Performance and Cost Models for a Second Generation Pressurized Fluidized Bed Combustion System," Morgantown Energy Technology Center, Morgantown, WV.

Frey H. C. and E. S. Rubin, 1992a, Evaluation of Advanced Coal Gasification Combined-Cycle Systems under Uncertainty, *I&EC Res.*, **31**, 1299.

Frey H. C. and E. S. Rubin, 1992b, Integration of Coal Utilization and Environmental Control in Integrated Gasification Combined Cycle System, *Env. Sci. Tech.*, **26**, 1982.

Frey H. C., E. S. Rubin, and U. M. Diwekar, 1994, Process Modeling of Advanced Technologies Under Uncertainty, *Energy*, **19** (4), 449.

Table 1. Uncertain Model Parameters for Illustrative Case Studies

DESCRIPTION AND UNITS (a)	Val (b)	Type	Min	Max	Prob.
Gasifier Fines Carryover,	5.0	F	0.0	1.0	5%
wt-% of Coal Feed			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,	95	F	50	90	25%
wt-% of Fines Carryover			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.

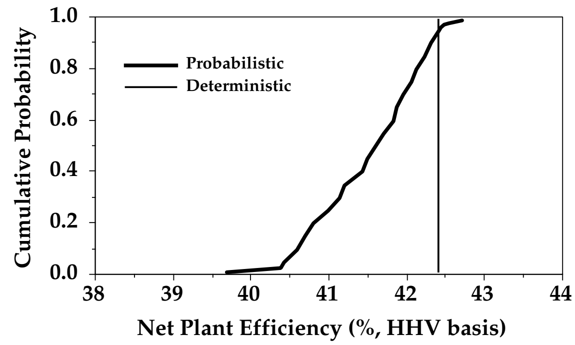

Figure 1. EFCC Plant Efficiency

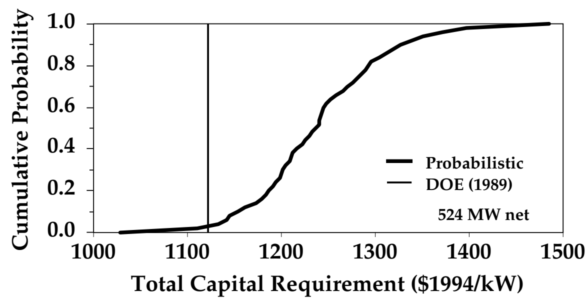

Figure 2. Second Generation PFBC System Total Capital Cost

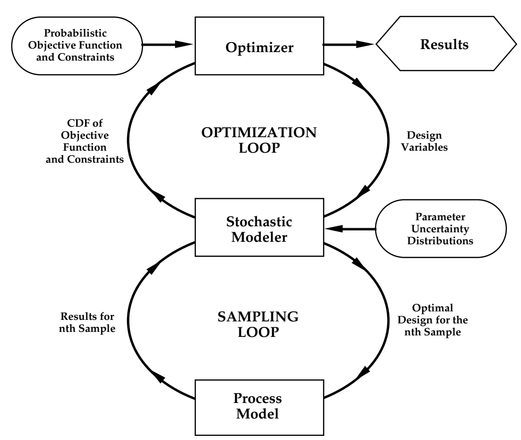

Figure 3. Schematic of the Stochastic Optimization Framework

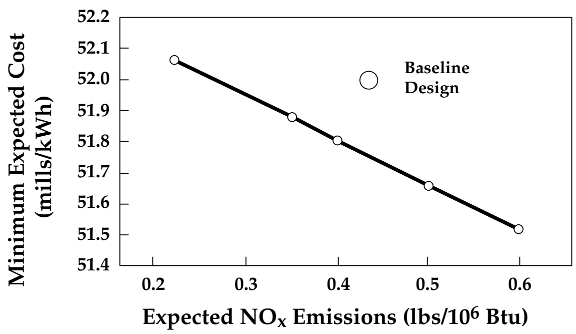

Figure 4. Minimize Total Cost Subject to NO_x Emission Constraint

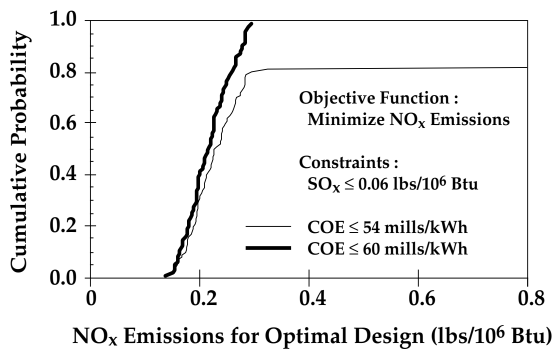

Figure 5. Minimize NO_x Subject to a Cost Constraint

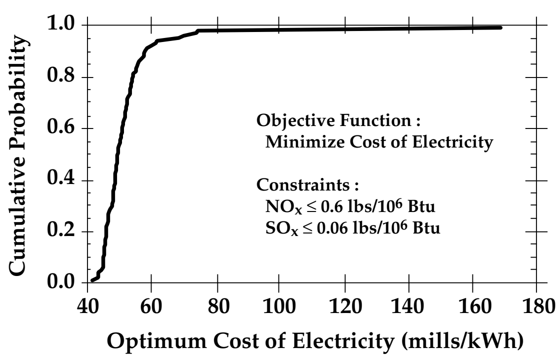

Figure 6. Effect Of Uncertainties on Cost of Optimal Design

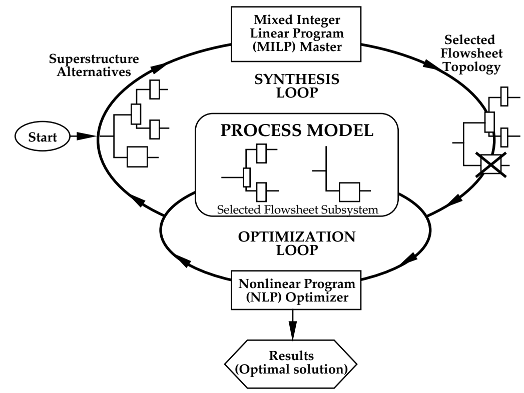

Figure 7. Schematic of the MINLP Synthesizer Framework

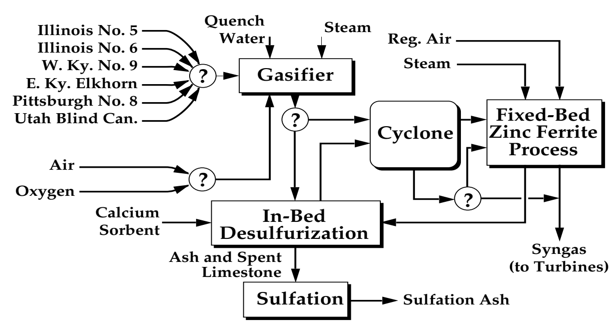

Figure 8. Synthesis of IGCC System