Designing Advanced Energy Systems Under Uncertainty

Urmila M. Diwekar and Edward S. Rubin

Department of Engineering and Public Policy
Center for Energy and Environmental Studies
Carnegie Mellon University
Pittsburgh, Pennsylvania 15213
Ph: (412) 268-5897; Fax: (412) 268-3757; rubin@cmu.edu

Abstract

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

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. 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.

The United States Department of Energy (DOE) has developed computer-based performance models for several IGCC systems using the Aspen process simulator. 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. Frey and Rubin (1992) extended the earlier DOE work to include new process performance models for environmental control systems, plus 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. Until now, each flowsheet was evaluated separately. However, as the number of technological options increases, an exhaustive search through individual flowsheet simulations to identify an optimal design configuration becomes computationally expensive. Thus, a systematic, efficient procedure for screening alternatives, and selecting an optimal design configuration, is desirable.

In this paper, the problem of identifying an optimal design configuration 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 traditional deterministic 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). These approaches, although different in principle, all provide useful directions for process synthesis research.

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 determines the discrete and continuous decision variables, where discrete variables denote the existence or absence of specific units in the flowsheet, and continuous variables represent flows, operating conditions, and design parameters of 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 Optimization Capability

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. Process *optimization* under uncertainty adds further complexity. 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.

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). 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 is 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 used 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. 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.

Process Synthesis Capability

To extend the modeling framework to include process synthesis, a process "superstructure" is added which includes all of the alternative flowsheet structures under consideration. The presence or absence of superstructure components thus determines a particular flowsheet. The process synthesis environment then consists of the two loops shown in Figure 2.

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. This new process synthesizer has been linked with the public version of the Aspen process simulator used by DOE. Additional details 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

The new process synthesis capability is illustrated in the context of a design decision for an IGCC power plant. A typical plant consists of three major sections: gasification, gas cleanup, and power generation. IGCC systems are classified primarily on the type of gasifier technology, oxidant, and gas cleanup method. Since U.S. coals have a wide range of properties that affect the thermal, environmental, and economic performance of IGCC systems, coal choice also is an important design variable.

Different combinations of coals, gasifiers, oxidants, emission control systems, and power generation equipment can give rise to a large array of different system configurations. 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. Since this study represents a first attempt to synthesize an IGCC flowsheet in the presence of uncertainties, the problem formulation was kept relatively simple in order to demonstrate the method, and to illustrate the computational efficiency achievable. The case study thus seeks to identify the optimal design configuration based solely on a choice of coal type and oxidant feed, involving a total of twelve different options.

Case Study Assumptions

The IGCC system modeled in this study employs the KRW gasifier, which is a pressurized fluidized-bed system. Steam plus air or oxygen react with coal to form a fuel gas stream containing CO, CO_2, CH_4, H_2, H_2S, COS, and NH_3. In-bed desulfurization may be performed using limestone or dolomite, which combines with sulfur to form calcium sulfide that is oxidized in a sulfation unit to form calcium sulfate. The fuel gas stream exiting the gasifier passes through ceramic cyclone filters which remove particulates. The gas then enters a desulfurization section where hydrogen sulfide is selectively adsorbed in a fixed bed of zinc ferrite pellets at 593C° (1100°F). The sulfided sorbent is regenerated using air as the oxidant and steam as the diluent. The regeneration off-gas containing SO_2 is then recycled to the gasifier. The clean fuel gas is burned in a gas turbine to produce power. Additional power is obtained from steam generated by the hot combustion gases exiting the turbine (Frey and Rubin, 1992).

The plant modeled is a nominal 700 MW facility operating at an annual capacity factor of 80 percent. An overall schematic of the plant is shown in Figure 3. Values of process performance and cost parameters, as well as key uncertainties, have been characterized in previous work (Frey et al., 1994). The uncertainty estimates shown in Table I were based on literature reviews, data analysis, and expert judgments of DOE process engineers based on the KRW IGCC system with hot gas cleanup. Six bituminous coals were analyzed (Table II).

The case study focused on options for coal choice and desulfurization. The superstructure for the case study is shown in Figure 4. Although in-bed and gas stream desulfurization are shown as discrete options, previous studies showed that the combination of these two technologies yielded the best economic performance (Diwekar and Rubin, 1992b). Therefore, only this option was included in the current flowsheet analysis. The optimization problem, based on expected values, was to minimize the expected cost of electricity for the overall plant subject to a maximum sulfur dioxide emission rate of 0.015 lbs/10^6 Btu. 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 III summarizes key results from the analysis. The numbers shown are the mean values of the probabilistic result for each case. One sees that the overall plant 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. Total plant 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.

The effect of uncertainties is illustrated in Figure 5, which show the cumulative distribution function (CDF) for the total capital cost, for the least-cost and highest-cost system configurations. The CDF 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). Since computer optimization methods 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. Figure 6 shows the probabilistic result for COE. The solid vertical line shows results from the deterministic analysis. The CDF shows 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. 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 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 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

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. Results were compared to those from the new process synthesis approach. 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. The stochastic synthesis approach demonstrated in this paper provides an efficient method for screening a large number of alternatives to identify the optimal design configuration in the face of uncertainties. Future work will extend this analysis to include a larger number of flowsheet options for advanced energy systems design.

Acknowledgements

This work was supported under Contract No. DE-AC21-92MC29094 from the U.S. Department of Energy's Federal Energy Technology Center. The authors alone, however, are responsible for the assumptions and results presented in this paper.

References

1. Chaudhuri, P., and U.M. Diwekar (1996), Synthesis under uncertainty: A penalty function approach, *AIChE Journal*, **42**, 742.
2. Diwekar, U.M. and J.R. Kalagnanam (1997), An efficient sampling technique for optimization under uncertainty, *AIChE Journal*, **43**, 440.
3. Diwekar, U.M., and E.S. Rubin (1991), Stochastic modeling of chemical processes, *Comput. Chem. Engng.*, **15,** 105.
4. Diwekar, U.M. , H.C. Frey, and E.S. Rubin (1992b), Synthesizing optimal flowsheets: Applications to IGCC system environmental control, *Ind. Eng. Chem. Res.* , **31**, 1927.
5. Douglas, J.M., *Conceptual Design of Chemical Processes*, McGraw-Hill, New York (1988).
6. Frey, H.C., and E.S. Rubin (1992), Integration of coal utilization and environmental control in integrated gasification combined cycle systems, *Environ. Sci. Technol*, **26** (10), 1982.
7. Frey, H.C., E.S. Rubin, and U.M. Diwekar (1994), Modeling uncertainties in advanced technologies: Application to a coal gasification system with hot gas cleanup, *Energy*, **19**(4), 449.
8. Friedler F., J.B. Verga, and L.T. Fan (1995), Algorithmic approach to the integration of total flowsheet synthesis and waste minimization, *Chemical Engineering Science*, **50**, 1218.
9. Grossmann, I.E. (1985), Mixed-integer programming approach for the synthesis of integrated process flowsheets, *Comput. Chem.Engng*, **9**(5), 463.

10. Longwell, J., E.S. Rubin, J. Wilson (1995), “Coal: Energy for the Future,” *Progress in Energy and Combustion Science*, Vol. 21, p. 269-360.
11. Narayan, V., U.M. Diwekar, and M. Hoza (1996), Synthesizing optimal waste blends, *Industrial & Engineering Chemistry Research*, **35**, 3519.
12. Nishida, N., G. Stephanopoulos, and A. Westerberg (1981), A review of process synthesis, *AIChE*, **27**, 321.
13. Painton, L. A., and U.M. Diwekar (1995), Stochastic annealing under uncertainty, *European Journal of Operations Research*, **83**, 489.

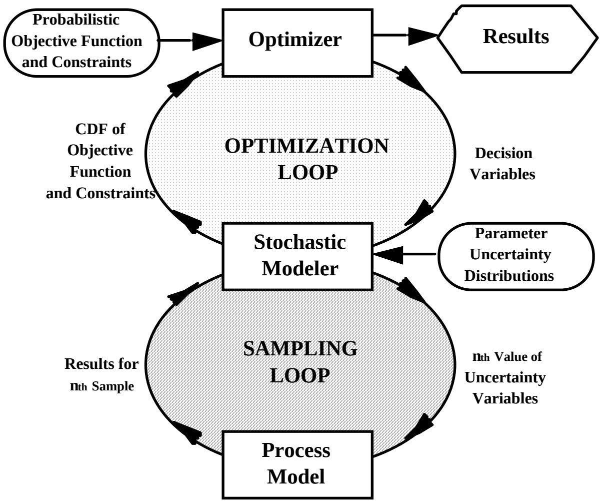

Figure 1. Stochastic optimization framework

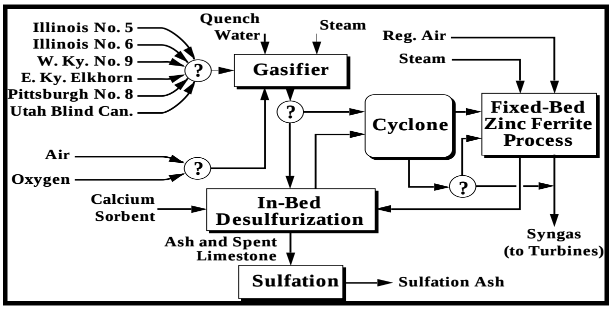

Figure 4. Schematic of flowsheet superstructure for IGCC case study

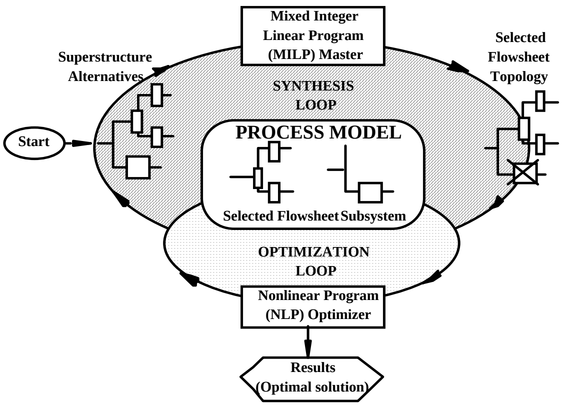

Figure 2. Process synthesis framework

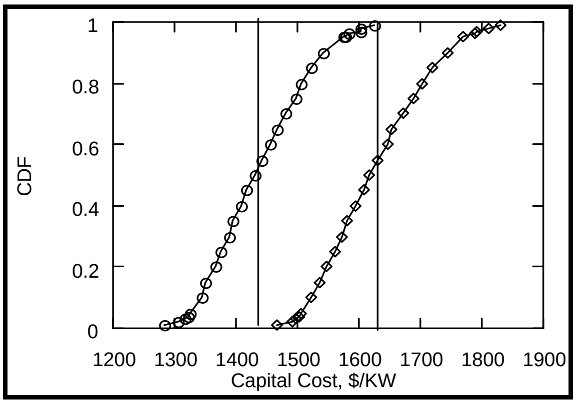

Figure 5. Total capital cost for the most and least expensive configurations

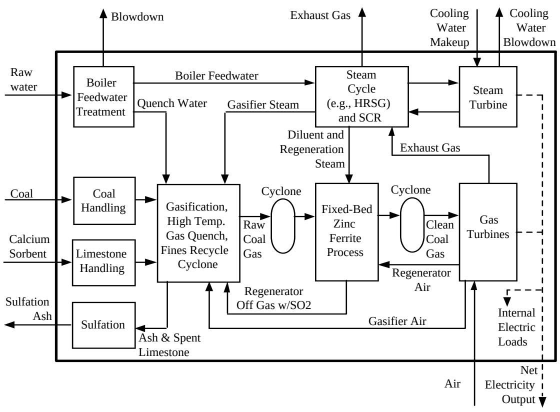

Figure 3. Simplified schematic of IGCC system (KRW gasifier with in-bed and hot gas desulfurization)

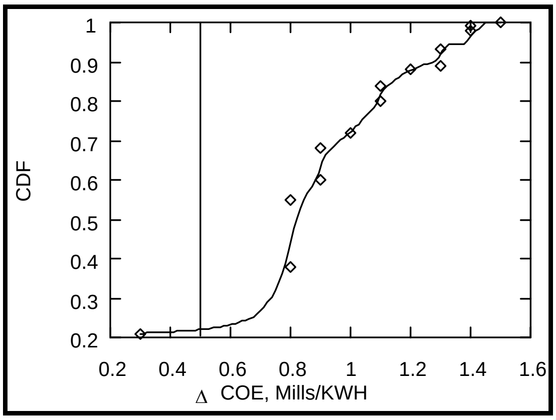

Figure 6. Cost of electricity difference for the two lowest cost systems

Table I. Uncertainty assumptions for case study

Parameter	Det. Value[a]	Probabilistic Value[b]
PERFORMANCE		
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_3 to NO_x	90	T: 50, 90, 100
Thermal NOx conversion, fraction air N fixated x 10^5	4.25	U: 1.0, 7.5
Gasifier NH3 yield, % of coal N	10	T: 0.5, 10, 10
Conversion of CaS to $CaSO_4$, %	60	U: 30, 90
Gas tubine CO conversion, wt % CO in fuel gas	98.85	U: 97.72, 99.99
COST PARAMETERS		
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

[a]Deterministic (nominal) value
[b]T=triangular dist (min, mode, max); U=uniform dist (min,max); N = normal dist (range shown is three standard deviations about the mean)

Table II. Coal properties for case studies

Parameter	Ill. 5	Ill. 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
HHV (Btu/lb)	13,250	12,774	12,245	13,524	13,760	14,140
Price ($/MBtu)	1.368	1.368	1.601	1.601	1.672	1.341

Table III. Mean value results for optimal process configuration using air (oxygen)[a]

Parameter	Ill.#5	Ill.#6	Ky	E.Ky.	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)

[a]Numbers in parenthesis refer to the oxygen-blown systems.