

A Process Analysis Approach to Pollution Prevention

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Technical and economic uncertainties are not rigorously treated or characterized in most preliminary cost and performance estimates of integrated environmental control technologies. Nor do current design methods rigorously address the issues of optimization under uncertainty. Furthermore, the process economics and a number of other quality measures, such as controllability, safety, compliance with environmental and other regulations, largely depend on the results of process synthesis stage. This conceptual design stage involves identifying the basic flowsheet structures to be used from a typically large number of alternatives. This paper describes the advanced computer-based methods for dealing with uncertainties that are critical to process viability, and for incorporating such factors into the synthesis and optimized design of advanced environmental control systems. Preliminary results are presented illustrating the use of these new modeling tools for the environmental control design of advanced integrated gasification combined cycle systems using hot gas cleanup.

INTRODUCTION

Increasing environmental awareness and regulations coupled with soaring waste management costs have created the need to incorporate more environmental considerations into the design and operation of industrial chemical processes. These environmental objectives have placed new requirements on process data and models, as well as increased the need for sophisticated simulation technology to quantify the impact of pollution prevention options.

In the 1970s, the design of environmentally compatible manufacturing plants generally meant the use of end-of-pipe treatment or separation devices through which effluent gases or liquids would pass on their way to the environment. Since then, a movement has grown that stresses waste reduction or pollution prevention during the early design stages of a process, and the concept of integrated environmental control has been gaining significant attention. The fundamental difference between conventional modeling and the new alternative of integrated environmental technologies, is the problem of uncertainties, since the available performance data are scant and the technical as well as the economic parameters are not well established. Moreover, many of the environmental processes are poorly understood and accurate predictive models do not exist. A framework for uncertainty analysis promises to provide an answer to these questions.

Though design under uncertainty has received considerable attention in the chemical engineering literature during the

past few years (Pistikopoulos and Grossmann, 1988; Straub and Grossmann, 1990; Varvarezos et al., 1993; Ciric and Huchette, 1993), a generalized framework for analyzing uncertainty systematically has only recently been developed around a chemical process simulator (Diwekar and Rubin, 1991). This capability has been used successfully for the evaluations of different configurations of "Integrated Gasification Combined Cycle Systems" (IGCC) which represent a clean and efficient use of coal (through reduction of NO_x and SO₂) for electric power generation (Frey et al., 1993). Currently this capability is centered around the public version of the ASPEN steady-state simulator. However, the methodology is general and could be extended to any other simulation environment. The first section of this paper will briefly discuss the methodology.

The trend in stochastic modeling is also reflected in the "stochastic optimization" and "stochastic programming" literature. Most of the work in this area is restricted to small scale linear and nonlinear programming problems of specific forms (Nemhauser et al., 1990; Ross, 1983; Davis and Vinter, 1985). Many of these solution techniques involve a highly formalized structure, require certain distributions on the random uncertainties or restrictions on the form of the objective function, often require convexity of the feasibility set and quasi-concavity of the probability measure, and typically do not involve large numbers of varying quantities. Furthermore, the stochastic optimization and stochastic programming literature very often divides the problems into categories such as "wait and see", "here and now" and "chance constrained optimization".

" (Vajda, 1972; Nemhauser et al., 1990). The "wait and see" problem of Madansky (1960), originally called "stochastic programming" by Tintner (1955), is in a sense not one of decision analysis. In decision making, the decisions have to be made "here and now" about the activity levels. In "wait and see" we wait until an observation is made on the random elements, and then solve the deterministic problem for each sample. The "here and now" problem, also referred to as the "stochastic optimization" problem, involves optimization over some probabilistic measure — usually the expected value. In that sense, chance constrained optimization problems can be included in this category of stochastic optimization. Chance constrained optimization involves constraints which are not expected to be always satisfied, but only in a proportion of cases, or "with given probabilities." The literature on chemical process design under uncertainty also involves problems like multiperiod optimization (Helman, 1979), and design for optimal flexibility (Grossmann et al., 1983; Straub and Grossmann, 1990) etc. These various categories require different methods for their solution.

This paper describes a framework for solving different stochastic optimization and stochastic programming problems. At first, the various problems reported in the literature on stochastic optimization/programming, and chemical process design under uncertainty are divided into two categories: 1) Stochastic optimization, and 2) Stochastic programming. The "here and now" problems involving expected value minimization, the chance constrained optimization problem, and the design for optimal flexibility problems all require that at each optimization iteration some probabilistic representation of the objective function and constraints to be optimized. These problems are classified as stochastic optimization problems. On the other hand, the "wait and see," "flexibility index," and multiperiod optimization problems involve solution of a deterministic optimization problem for each scenario so that one gets a probabilistic representation of optimal solutions. Therefore, these type of problems can be considered under the second category namely that of stochastic programming. This new division makes it easier to generalize the use of this new capability for different kinds of optimization problems under uncertainty and to design a uniform framework for solving large scale problems. The second section describes these two categories in detail. The generalized framework designed around the public version of ASPEN simulator is presented, followed by solution to stochastic optimization and stochastic programming problems encountered in a hot gas cleanup integrated gasification combined cycle (IGCC) system.

Integrated environmental control processes may employ alternative paths and raw materials to reach the desired product. One of the major goals in process synthesis is to establish methodologies for determining optimal flowsheet configurations. The research in chemical process synthesis has advanced considerably in last few decades and a number of packages now provide an environment for solving synthesis problems (CPS, 1993, APROS (Paules and Floudas, 1989), DICOPT++ (Kocis and Grossmann, 1989; Viswanathan and Grossmann, 1990), PROSYN (Kravanja and Grossmann, 1990)). However, these

packages have some practical limitations; for example, it may be too cumbersome and time consuming to handle complex chemical processes such as those typically encountered in a realistic plant.

Sequential-modular simulators like ASPEN and PRO/II, have grown in sophistication over the years and are widely used in the chemical industries to solve complex problems with rigorous process modeling. Therefore, it is more desirable to build the process synthesis capability around such simulators. A new process synthesis capability built around the public version of ASPEN simulator (Diwekar et al., 1991) represents a step in this regard. The third section of this paper will be devoted to describing this mixed integer nonlinear programming (MINLP) process synthesizer built around the ASPEN simulator and demonstrating its use via an illustrative case study of a complex environmental flowsheet. However, the MINLP approach to process synthesis also encounters some difficulties when faced with the problems of nonconvexities, large discontinuities, local minima, and implicit constraints.

The alternative to MINLP process synthesis is to use simulated annealing. Although simulated annealing is computationally intensive to MINLP synthesis, it circumvents the problems associated with MINLP synthesizer. Furthermore, a new algorithm "stochastic annealing" (Painton and Diwekar, 1994; Chaudhuri and Diwekar, 1994a,b) is developed which efficiently optimizes a probabilistic objective function. Section four briefly describes this new algorithm and its applicability. The essence of the paper is presented in the last section on conclusions.

A PROBABILISTIC FRAMEWORK FOR UNCERTAINTY ANALYSIS

A new stochastic modeling capability has been added to the public version of ASPEN by Diwekar and Rubin (1991). To implement the stochastic modeling capability, ASPEN's modular nature has been utilized. A new unit operation block STOCHA has been added to the ASPEN unit operation library. The structure of the block and its use are briefly described below. Details are provided elsewhere (Diwekar and Rubin, 1991).

The stochastic module assigns the probabilistic distribution to the model input parameters, then uses a sampling technique to generate a specified number of samples and passes the sampled value of each parameter to the model. After each model run, the output variables of interest are collected. The simulation is then repeated for a new set of samples selected from the probability distributions. After all the samples have gone through the cycle, the stochastic module analyzes the output and presents the likelihood of the outcome in terms of probabilistic distributions. It also provides the sensitivity analysis information in terms of partial correlation coefficients and standardized regression coefficients.

In stochastic modeling, the uncertain or variable parameters in the model are expressed in terms of probability distributions. These probability distributions show the range of values

the variable could take and the likelihood of occurrence of each value within the range. Thus, the distribution defines the rule for describing the measures associated with the values of a random (uncertain) variable. Probability distributions may be described in their entirety as cumulative distribution functions, or by selected parameters, such as fractiles and moments (e.g. mean, variance). A more complete review of these methods may be found in Morgan and Henrion (1990).

As can be envisioned from the steps outlined above, the stochastic modeling (depending on the number of samples) may require large computational efforts. The computationally intensive nature of such analysis makes the research to refine the sampling technique very important especially when one is solving problems like stochastic optimization and stochastic process synthesis.

There are many ways of sampling from probability distributions, of which the best known is *Monte Carlo Simulation*. In crude Monte Carlo analysis, sample values are drawn at random from the distributions of each input variables. It is often not realized that the value of the Monte Carlo methods is not primarily the randomness of the sampling but the resulting equidistribution properties of the sets of points in the parameter space. Once it is recognized that a primary objective is to produce a more uniform distribution of points in space, then systematic or stratified sampling techniques become appealing (Morgan and Henrion, 1990). Latin Hypercube Sampling (LHS) (Iman and Shortencarier, 1984) which represents a form stratified sampling is often used to provide better uniformity properties and is available with the stochastic block.

Research is also being carried out to improve the uniformity of sampling techniques and a new and more efficient sampling technique based on Hammersley points has emerged from these efforts (Kalagnanam and Diwekar, 1994).

METHODOLOGY FOR STOCHASTIC OPTIMIZATION AND STOCHASTIC PROGRAMMING

The probabilistic framework outlined earlier can not only be used for getting the likelihood of an outcome, but can also provide a basis for research prioritization, comparison of different technologies, feasibility studies, risk analysis etc. This stochastic modeling capability, along with an optimizer, can solve different stochastic optimization and stochastic programming problems, as discussed below.

The Optimizer

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

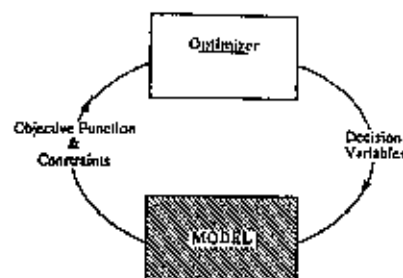


Figure 1: Pictorial Representation of the Optimization Framework

equation,

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

$$x$$

subject to

$$h(x) = 0 \quad (2)$$

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

where x is a decision variable vector. The above formulation represents the deterministic optimization problem, for which a generalized iterative solution procedure is illustrated schematically in Figure 1. As seen in the figure, the optimizer invokes the model with a set of values of decision variables x . The model simulates the phenomena and calculates 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 pertaining to the optimization algorithm are satisfied. In this case the model which is used is deterministic in nature.

The optimizer block, OPTM, has been implemented in ASPEN as a unit operation block. The OPTM block is a flowsheet optimization block which solves the nonlinear optimization problem (NLP) described above.

Recent advances in constrained nonlinear optimization techniques provide better choices for solving large scale flowsheet problems. The most popular of these methods are generalized reduced gradient (GRG) and successive quadratic programming (SQP), and their variants. Among generalized reduced gradient methods, the most widely used algorithms are GRG2 and MINOS (Gill et al., 1981). Most literature on large scale optimization favors the SQP method because the GRG2 algorithm requires convergence of equality constraints at each iteration. In SQP, at each iteration the problem is approximated as a quadratic program where the objective function is quadratic and the constraints are linear. Similar to linear programming, the special features of a quadratic objective function are exploited to solve the problem more efficiently. The quadratic programming subproblem is solved for each step to obtain the next trial point. This cycle is repeated until the optimum is reached. The NLP optimization block in ASPEN

OPTM, generates decision variable sets using the SQP method (Biegler and Cuthrell, 1985). The modular nature of both the stochastic and optimization blocks allow one to solve different stochastic optimization and stochastic programming problems encountered in practice. The following subsection describes this functionality.

Stochastic Optimization

In many cases, including advanced integrated control technologies, the model builder cannot ignore the uncertainties associated with some of the model input parameters. An uncertainty analysis thus becomes essential. As uncertainty is a broad concept, it is possible—and often useful—to approach it in several different ways. One rather general approach, which has been described earlier (see section 1) and successfully applied to a wide variety of problems, is to assign a probability distribution to the various uncertain or variable parameters.

The generalized stochastic optimization problem, where the decision variables and uncertain parameters are separable, can then be viewed as:

$$\text{Optimize } J = F_1(j(\theta, x, u)) \quad (4)$$

θ

subject to

$$F_2(h(\theta, x, u)) = 0 \quad (5)$$

$$F_3(g(\theta, x, u) \leq 0) \geq \alpha \quad (6)$$

where u is the vector of uncertain parameters and the F represents the cumulative distribution functional which for an expected value minimization reduces to:

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

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

$$E(F(u)) = \frac{\sum_{i=1}^{N_{\text{sample}}} F(u)}{N_{\text{sample}}} \quad (8)$$

On the other hand, in the case of chance constrained optimization the constraints are represented in terms of a probability of exceeding certain value and is represented by:

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

x

subject to

$$P(h(x, u) > \beta) \leq P_c \quad (10)$$

where Equation 10 is the chance constraint.

It is apparent from the above discussion that 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 the deterministic model inside the optimization loop. The

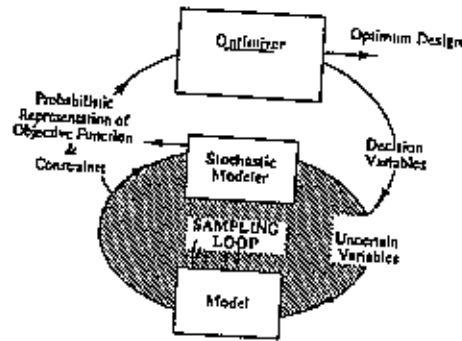


Figure 2: Pictorial Representation of the Stochastic Optimization Framework

number of samples required to obtain the accurate probabilistic functional depends on various factors. The accuracy of these estimates is discussed in the context of synthesis under uncertainty.

Figure 2 represents the generalized stochastic optimization problem solution procedure where the deterministic model in Figure 1 is replaced by an iterative stochastic model. Figure 3 illustrates the ASPEN implementation.

This stochastic optimization capability can also be used to achieve off-line quality control. In off-line quality control, the sensitivity of the design to the sources of variation is reduced at the design stage to make the controller design easier. One such approach based on the concept of Taguchi's parameter design method has been illustrated using the above-mentioned stochastic optimization capability (Diwekar and Rubin, 1994). This approach involves minimizing the variance of the objective function instead of the expected value.

Effect of Uncertainties on Optimal Design

In contrast to the stochastic optimization problems, which involve expected value minimization, and the chance constrained problems etc., the "wait and see," and multiperiod optimization problems are categorized as stochastic programming problems. The "wait and see" problem involves deterministic decisions at each random stage or random sample, which is the same as solving multiple deterministic optimization problems, and can be represented as:

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

x

subject to

$$h(x, u^*) = 0 \quad (12)$$

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

where u^* is the vector of values of uncertain variables corresponding to some sample. This optimization procedure is

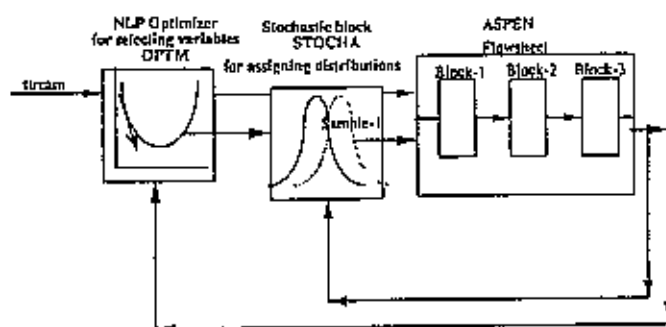


Figure 3: Schematic of ASPEN Stochastic Optimization Framework

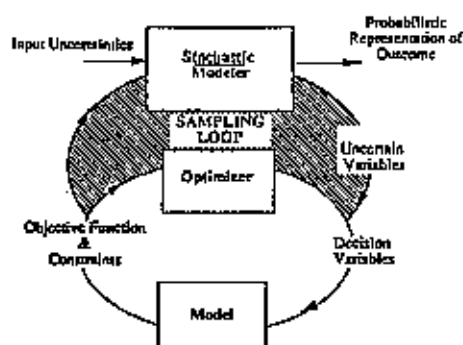


Figure 4: Pictorial Representation of the Stochastic Programming Framework

repeated for each sample of uncertain variables u and a probabilistic representation of outcome is obtained. Figure 4 represents the generalized solution procedure where the deterministic problem shown in Figure 1 forms the inner loop, whereas the stochastic sampling forms the outer loop. This procedure is implemented in the ASPEN simulator as shown in Figure 5. From the ASPEN representation, it is clear that by just interchanging the position of stochastic block, STOCHA, and the optimization block, OPTM, one can solve almost all the problems in the stochastic optimization/programming literature.

METHODOLOGY FOR THE PROCESS SYNTHESIS CAPABILITY

The alternatives for process design often are numerous and involve a very large search space. Selection of the best alternatives can offer the potential for significantly reducing costs and/or improving performance. Therefore, there is a strong

need for "systems" research to identify the best ways of configuring environmental control processes. The current state of process synthesis techniques involves: (a) the heuristic approach which relies on intuition and engineering knowledge, (b) the physical insight approach which is based on exploiting basic physical principles, and (c) the optimization approach which uses the mathematical programming techniques. This section deals with a newly developed process synthesizer built around the public version of ASPEN, using the mathematical programming approach (Diwekar et al., 1991).

The Mathematical Programming Approach

The mathematical programming approach to process synthesis involves:

- Formulation of a flowsheet superstructure incorporating all the alternative process configurations.
- Modeling the superstructure as a mixed integer nonlinear programming (MINLP) problem of the form

MINLP:

$$Z = \min_{\bar{x}, \bar{v}, \bar{y}} c^T \bar{y} + f(\bar{x}, \bar{v}) \quad (14)$$

subject to

$$\begin{aligned} h(\bar{x}, \bar{v}) &= 0 \\ h1(\bar{x}, \bar{v}) &= v - x(\bar{x}) = 0 \\ B^T \bar{y} + g(\bar{x}, \bar{v}) &\leq 0 \\ y &\in Y; x \in X \end{aligned} \quad (15)$$

where

$$\begin{aligned} Y &= \{y | Ay \leq a, y[0, 1]^m\} \\ X &= \{x | x^L \leq x \leq x^U\} \end{aligned}$$

The continuous variables x represent flows, operating conditions, and design variables. The variables v are the

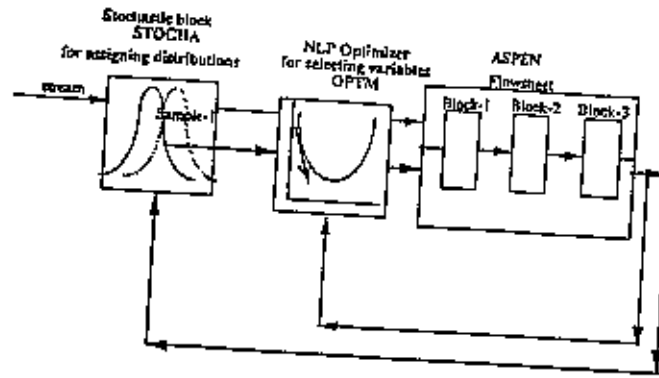


Figure 5: Schematic of the ASPEN Stochastic Programming Framework

output variables which are related to the input variables x by model equations. For equation oriented environments, these model equations are embedded in the equality constraints $h1(\bar{x}, \bar{v})$. The binary variables y denote the potential existence of process units.

- (c) Identification of both the optimal configuration and operating process parameters by an algorithm based on alternating sequence of nonlinear programs (NLPs) and mixed integer linear programs (MILPs).

The ASPEN MINLP Process Synthesizer

The MINLP process synthesis capability in the public version of ASPEN is based on ZOOM (Marsten, 1986), the mixed integer linear programming (MILP) solver, and on SCOPT (Lang and Biegler, 1987), the nonlinear programming (NLP) solver. The method is based on an algorithm called GBD/OA/ER/AP presented by Diwekar et. al (1991) which involves solution of alternate sequence of MILP and NLP problem solving. The overall structure of the environment is shown in Figure 6. Optimization of the MINLP process synthesis problem is decomposed into continuous optimization of NLP problems at fixed choice of binary variables, and discrete optimization through the MILP master problem. The MILP solver (Master) and NLP optimizer have been implemented in ASPEN as unit operation blocks and can be executed easily with the ASPEN process unit blocks.

The process synthesis environment in ASPEN consists of the Master block, the NLP optimizer, and the entire superstructure. The initialization of the continuous and binary variables is done in the ASPEN input file. At this stage the scheme is translated into an initial flowsheet and subsystems using the decomposition strategy of Kravanja and Grossmann (1990). NLP optimization of the selected flowsheets is the first step in the inner loop, which results in the objective function and linearization information. This information is passed to the Master block which internally modifies the master problem to include the linearization information. The solution of the mas-

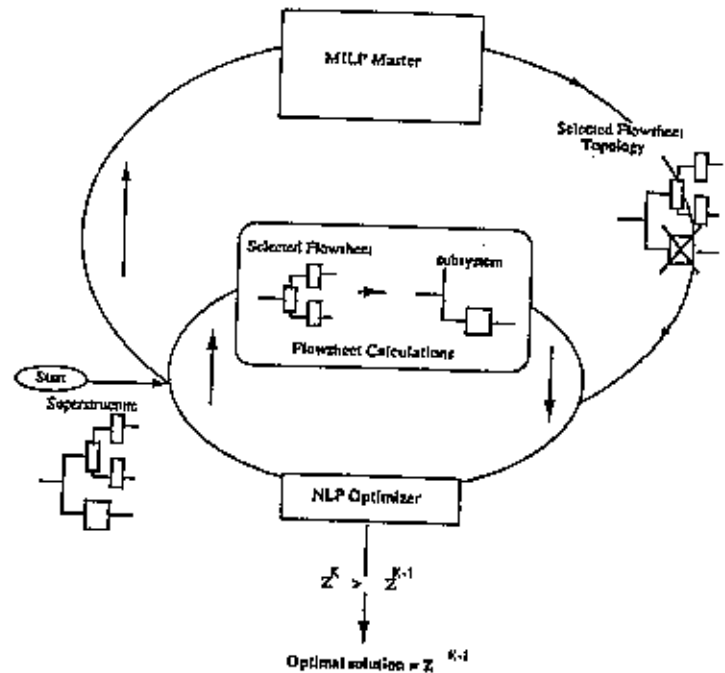


Figure 6: Schematic of the ASPEN MINLP Synthesizer

ter problem results in a new flowsheet structure. The iteration stops when there is no improvement in the objective function value.

The Implicit Constraint Problem

The implementation of this new capability in a sequential modular simulator poses challenging problems which are not encountered in equation-oriented simulators; therefore, new strategies are necessary to solve these problems. One such problem associated with the MINLP sequential modular process synthesizer is that of *implicit constraints*.

The problem of implicit constraints is encountered because of the black box nature of the models in sequential modular simulators. The ASPEN MINLP environment is based on a two-level optimization algorithm consisting of an upper level MILP master problem and a lower level NLP problem. The MILP master problem predicts new binary variables, while the NLP problem provides new continuous variables. The MILP master problem represents the linearized NLP problem with non-fixed binary variables, since at each stage the MILP master problem obtains the linearization information from the NLP optimizer. Unlike equation oriented simulators, in sequential modular simulators most of the nonlinear constraints are not represented explicitly by equations. The linearization information on these constraints, which are essentially black box relations embedded in the simulator environment ($h1(\bar{x}, \bar{v})$ in equation 2), therefore must be passed to the master problem.

In order to circumvent this problem of implicit constraints new decision variables are created. These are equated to the output variables from the flowsheet configurations. This procedure ensures that the original MINLP problem remains the same, while at each stage the MILP master problem receives increased information from the NLP optimizer. Although this procedure assures complete information transfer to the master problem, it also increases the computational load on the NLP optimizer, which is generally the rate-determining step in the MINLP process synthesis. Recently Diwekar and Rubin (1993) presented a partitioning strategy which reduces the computational load on the NLP problem crucial for the solution of large-scale synthesis problems.

Apart from the problem of implicit constraints, the MINLP process synthesis capability encounters difficulties when function does not satisfy convexity conditions, for systems having large combinatorial explosion, or when the solution space has discontinuities. Simulated annealing is a recently developed probabilistic method for combinatorial optimization based on ideas from statistical mechanics (Kirkpatrick et al. 1983). The advantages of simulated annealing are that it is not a derivative based method and can handle discontinuities in the state space much more easily. Hence it provides an alternative to MINLP synthesis. The synthesis problem usually involves discrete decisions and requires solution of combinatorial optimization problems. These problems are much more difficult to solve and computationally intensive than continuous optimization problems. The inclusion of uncertainty analysis in such large scale problems needs special

care to handle the combinatorial explosion as a result of sampling at each optimization step. The next section presents the stochastic annealing algorithm designed to efficiently optimize a probabilistic functional of the objective. The method is first developed for expected value of objective function (Painton and Diwekar, 1994) and further extensions of this method for other probabilistic functions is underway (Chaudhuri and Diwekar, 1994a, 1994b).

STOCHASTIC ANNEALING FOR SYNTHESIS UNDER UNCERTAINTY

The idea behind the stochastic annealing algorithm presented here is to allow the algorithm to select a trade-off between accuracy and computational efficiency. When the optimizer is still away from the optimum the efficiency is more important than accuracy and near optimum, the accuracy is given more weight so that the optimizer converges to an accurate optimal solution with minimum computational effort. This strategy also allows for automatic sample selection which otherwise requires extensive experimentation.

The Simulated Annealing Algorithm

The analogy in simulated annealing is to the behavior of physical systems in the presence of a heat bath: in physical annealing, all atomic particles arrange themselves in a lattice formation that minimizes the amount of energy in the substance, provided the initial temperature (T_{init}) is sufficiently high and the cooling is carried out slowly. At each temperature T , the system is allowed to reach thermal equilibrium, which is characterized by the probability (Pr) of being in a state with energy E given by the Boltzmann distribution:

$$Pr_E = \frac{1}{Z_t} e^{-\frac{E}{K_b T}} \quad (16)$$

where K_b is the Boltzmann constant (1.3806×10^{23} J/degreesK) and $\frac{1}{Z_t}$ is a normalization factor.

In simulated annealing, the objective function (usually cost) becomes the energy of the system. The goal is to minimize the cost/energy. Simulating the behavior of the system then becomes a question of generating a random perturbation that displaces a "particle" (moving the system to another configuration). If the configuration S representing the set of the decision variables θ that results from the move has a lower energy state, the move is accepted. However, if the move is to a higher energy state, the move is accepted according to the Metropolis criteria (accepted with probability $= \frac{1}{Z_t} e^{-\frac{E}{K_b T}}$) (vanLaarhoven and Aarts, 1987). This implies that at high temperatures, a large percentage of uphill moves are accepted. However, as the temperature gets colder, a small percentage of uphill moves are accepted. After the system has evolved to thermal equilibrium at a given temperature, the temperature is lowered and the annealing process continues until the system reaches a temperature that represents "freezing" ($T = T_{freeze}$). The

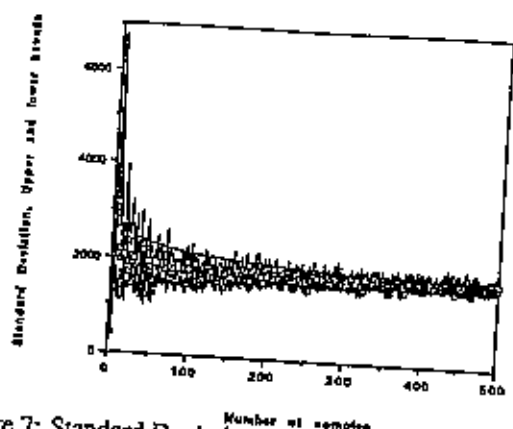


Figure 7: Standard Deviation versus Number of Samples

equilibrium detection at each temperature is a function of the maximum allowable moves at each temperature, N_T or accept reject limits N_{acc}/N_T . Thus simulated annealing combines both iterative improvement in local areas and random jumping to help ensure the system does not get stuck in a local optimum.

Penalty for Small Number of Samples

The major bottleneck in stochastic optimization problems is the computational time required to generate the probabilistic functional of objective function and constraints. Given m observations y_i of the random variable Y , the estimator for the mean or expected value (\bar{y}) and variance (σ_y^2) are:

$$\bar{y} = \frac{\sum_{i=1}^m y_i}{m} \quad (17)$$

$$\sigma_y^2 = \frac{\sum_{i=1}^m (y_i - \bar{y})^2}{m - 1} \quad (18)$$

The accuracy of any probabilistic functional depends upon number of samples. For example, Figure 7 shows how the standard deviation of simple function ($x_1 \times x_2$) of two variables x_1 (Uniform (10,20)) and x_2 (Normal(6.5,16.5)) is varying with number of samples for Random Monte Carlo Simulations. Central limit theorem offers an approximate bounds for predicting accuracy of these probabilistic functional. The solid lines in the Figure 7 represent these bounds. While the central limit theorem provides the estimates of precision of the expected values for given number of samples m for truly random sample (generated by Monte-Carlo Simulations), it provides a very loose upper bound on the error band for more uniform but less independent samples generated by Latin Hypercube Sampling and more research is needed to estimate this band width. An novel approach based on the concept of fractal dimension is being investigated.

In our stochastic annealing we have used this error width as a penalty in the objective function allowing stochastic annealing to manipulate the number of samples. The trade-offs between the accuracy (where the penalty weights are higher) and efficiency (fewer samples) are decided based on the annealing temperature. The details of the algorithm is described below.

The Stochastic Annealing Algorithm

The goal of stochastic annealing is to minimize a probabilistic function of the objective or cost function by balancing the trade-offs between accuracy and computational efficiency. In simulated annealing, the algorithm examines the (deterministic) cost function at one point in the configuration space, jumps randomly to another configuration and calculates the cost function of that point. Initially when one is away from the optimum the annealing algorithm accepts more uphill moves but as it approaches optimum it accepts less number of uphill moves. This strategy is implemented in terms of the cooling schedule and the metropolis criterion. In stochastic annealing the cooling schedule is also used to decide the weight on the penalty for imprecision in the expected functional. So, the new objective function used in stochastic annealing consists of probabilistic objective function value and the penalty term, and is represented for mean and variance functional as follows:

$$E(Z) = \frac{\sum_{i=1}^{N_{samp}} Z_i}{N_{samp}} + b(t) \frac{2\sigma_z}{N_{samp}^{1/2}} \quad (19)$$

$$\sigma_z^2 = \frac{\sum_{i=1}^{N_{samp}} (Z_i - \bar{z})^2}{N_{samp} - 1} + \frac{b(t)}{2} \left(\frac{(N_{samp} - 1)\sigma_z^2}{\chi_{0.025}^2} + \frac{(N_{samp} - 1)\sigma_z^2}{\chi_{0.975}^2} \right) \quad (20)$$

In these equations, the first term is the expected cost function and the second term is the penalty function where χ^2 represents the chi-square distribution.

The weighing function $b(t)$ can be expressed in terms of the annealing temperature levels. At high temperatures, it is not necessary to take a large number of samples to get an accurate expected cost because the algorithm is still exploring the entire configuration space to see where the optimal regions lie. However, as the system gets cooler and the algorithm "hones in" upon the optima, it is necessary to take more samples to get more accurate expected costs. Thus b is initially very small but increases with temperature decrease. We used an exponentially increasing function for b given by:

$$b(t) = \frac{b_0}{k^t} \quad (21)$$

where b_0 is a small value (for example, .01), k is a constant which governs the rate of increase (for example, .9) and t is the temperature level.

This algorithm was found to be 50 to 80 % faster as compared to the fixed sample annealing (Painton and Diwekar, 1994, Chaudhuri and Diwekar, 1994a, 1994b). The algorithm is especially attractive as it accurately chooses number of samples automatically.

ILLUSTRATIVE EXAMPLES

The new capabilities for MINLP process synthesis, stochastic annealing, and optimization under uncertainty provide powerful new tools for the design and analysis of advanced...

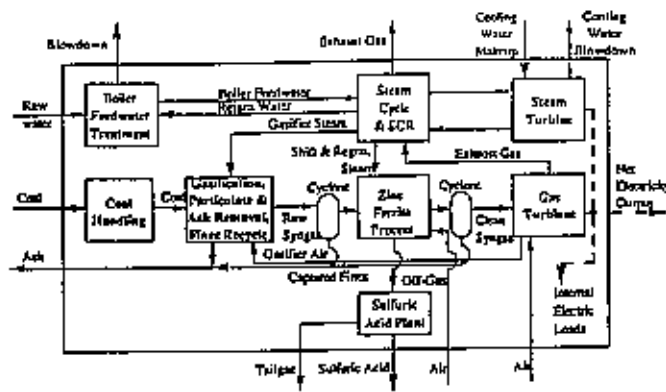


Figure 8: Schematic of the Lurgi Air-blown Dry Ash Gasifier IGCC System

control systems. An application of the synthesis capability already has been described in a paper (Diwekar, et al., 1992), which focuses on choosing a least-cost approach to sulfur removal for an IGCC system with hot gas cleanup and a fluidized bed gasifier. In this paper we show results that illustrate use of the stochastic optimization and stochastic programming capabilities for the design of a different IGCC system with objectives such as cost and emissions minimization, and risk reduction. These objectives also form the basis for synthesis under uncertainty. Number of case studies, related to advanced control technologies selection, using the efficient stochastic annealing algorithm are in progress (Chaudhuri and Diwekar, 1994a, 1994b). Although, this approach to solving stochastic optimization and stochastic programming problems is general and applicable to wide variety of problems, it can be computationally expensive.

To illustrate the stochastic optimization and programming capabilities, an air-blown dry ash Lurgi gasifier IGCC system flowsheet with a plant size of 650 MW and a high-sulfur Illinois No. 6 coal is analyzed. A schematic of this technology is shown in Figure 8. The hot gas cleanup system features high temperature (1100 degrees F) sulfur removal from the fuel gas with a zinc ferrite sorbent, and high efficiency cyclones and ceramic filters for particulate removal. Details of the performance and cost models are reported elsewhere (Frey and Rubin 1992a).

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. Another key area of uncertainty for this technology is the NO_x emission rate. 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 system are typically located in the heat recovery steam generator (HRSG). We employ a new performance and cost model of an SCR system (Frey, 1993) 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.

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. 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. A sample size of 25 was used to illustrate the new capabilities. For details the readers are referred to Diwekar et al. (1994).

Figures 9 to 13 show the results of different stochastic optimization and stochastic programming problems applied to the IGCC flowsheet.

Figure 9 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 value of NO_x emissions is decreased, the cost of the optimal design increases, as does the expected value of NO_x removal efficiency in the SCR unit. As seen in Figure 9, the optimal design reduces the expected COE by 0.5 mills/kWh relative to the base case design achieving 0.44 lbs $\text{NO}_x/10^6$ Btu. For the 650 MW plant modeled in this example, this is equivalent to a total savings of approximately \$2 million per year in plant costs resulting from the selection of optimal design parameters in the zinc ferrite and SCR units. Figure 9 also shows that the expected cost of the optimal design increases by 1.1 mills/kWh as NO_x is lowered from 0.6 to 0.2 lbs/ 10^6 Btu. Over this range, the optimal SCR removal efficiency increases from 73% to 90% (the maximum value established

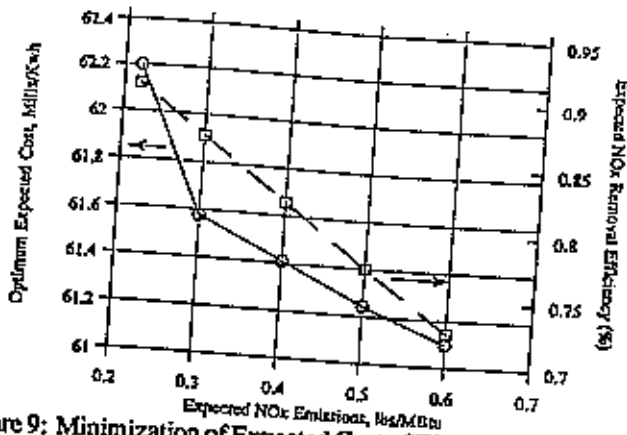


Figure 9: Minimization of Expected Cost of Electricity Subject to Expected Value of NO_x Emission Constraints

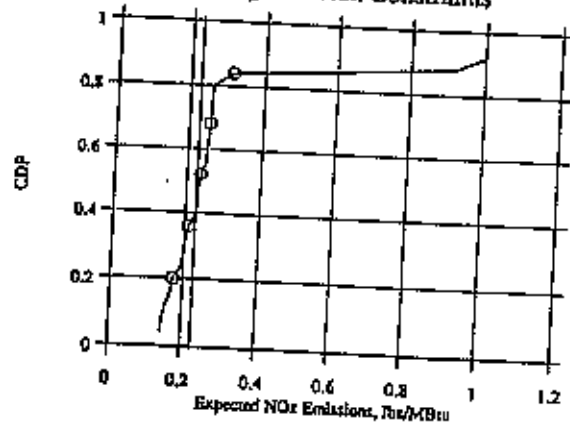


Figure 10: Effect of Uncertainties on Minimum Cost

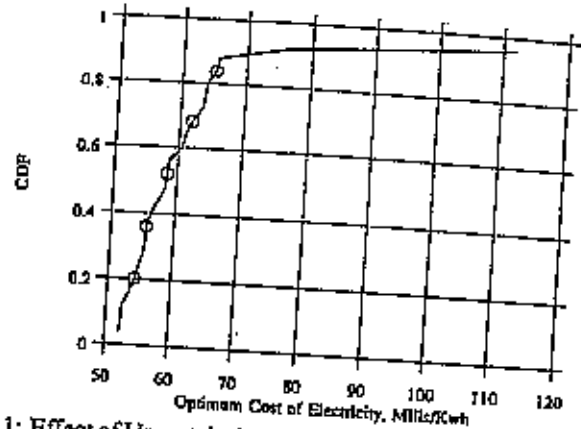


Figure 11: Effect of Uncertainties on Minimum NO_x Emissions

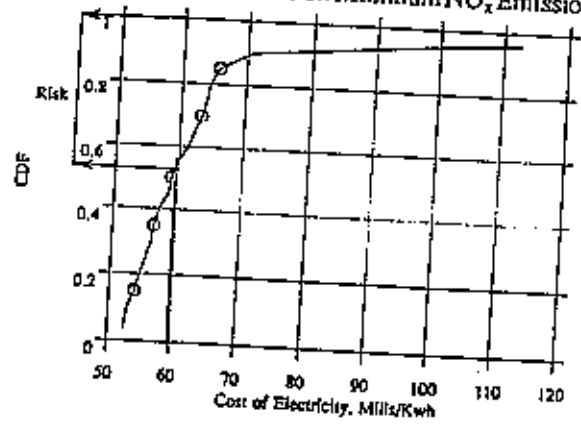


Figure 12: Risk as % Probability of Exceeding Cost Limit

by the performance model). This limits the lowest achievable NO_x emissions to 0.22 lbs/10⁶ Btu (expected value).

Figure 10 next shows the effect of uncertainties on the cost of an optimal design for the case of NO_x emissions constrained to 0.5 lbs/10⁶ Btu or less, and SO₂ emissions to 0.06 lbs/10⁶ Btu or less. The cost of electricity for the optimal design configuration varies by more than a factor of two due to the performance and cost uncertainties. An 80% confidence interval gives expected costs between 52.5 and 70.0 mills/kWh. Also there is a 5% probability of no feasible design able to meet the emission constraints with the assumed uncertainties.

Figure 11 shows an example in which NO_x emissions are minimized subject to a constraint on the maximum cost of electricity (in this case, 65 mills/kWh), representing an assumed upper bound on economic risk. The stochastic programming results for this case show a 50% probability of optimal designs achieving between 0.2 and 0.3 pounds NO_x/10⁶ Btu. The mean value of the probabilistic results show a minimum NO_x emission rate of 0.32 lbs/10⁶ Btu for this case. However, Figure 13 also shows a 15% chance of exceeding 0.6 lbs/10⁶ Btu, which is the Federal New Source Performance Standard (NSPS) for coal-fired power plants. Thus, reducing process uncertainties or modifying process configuration to reduce the level of risk may be warranted.

Finally, Figures 12 and 13 illustrate the concept of risk minimization. The risk can be defined as probability of exceed-

ing some specified value of cost. Figure 12, defines the risk as probability of exceeding the cost (of electricity) 60 mills/kWh. Then the problem is formulated as minimization of this risk subject to the chance constraint of probability of exceeding the NO_x emissions of 0.35 lbs/Btu is less than the different probabilities P_c. Figure 15 shows the minimum risk at different chance constraints P_c. It can be seen that the risk could not be minimized much. This may be because the decision variables selected are less sensitive to the risk.

These results are intended only to be illustrative of the new modeling capabilities now possible with stochastic optimization and stochastic programming. For realistic case studies, one

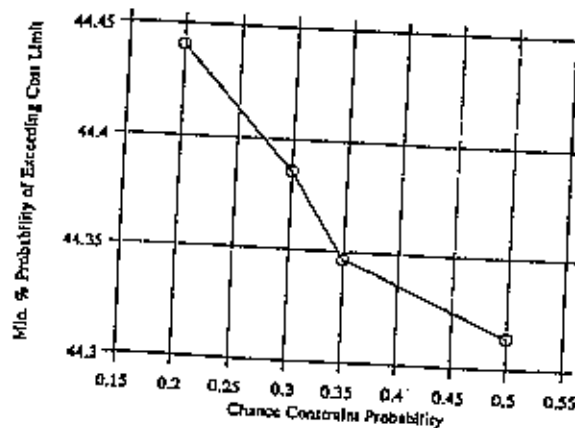


Figure 13: Risk Minimization

may need to consider a larger sample size or switch to more efficient sampling techniques such as described by Kalagnanam and Diwekar (1994).

CONCLUSIONS

This paper has presented new systems analysis tools and methodologies that can substantially improve the design and analysis of environmental control technologies. By combining existing process simulators with the mathematical methodologies presented here (i.e., probabilistic modeling, optimization, MINLP synthesis, and stochastic annealing) researchers now can tackle a wide range of system performance and cost analysis not heretofore possible. Furthermore, this toolbox can be used to insure that environmental issues are fully considered in all phases of process engineering activity, ranging from synthesis to design to operations. 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 issues.

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