Stochastic modeling and multi-objective optimization for the APECS system

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**Abstract**

The Advanced Process Engineering Co-Simulator (APECS), developed at the U.S. Department of Energy's (DOE) National Energy Technology Laboratory, is an integrated software suite that enables the process and energy industries to optimize overall plant performance with respect to complex thermal and fluid flow phenomena. The APECS system uses the process-industry standard CAPE-OPEN (CO) software standard to combine equipment models and commercial process simulation software with powerful analysis and virtual engineering tools. The focus of this paper is the CO-compliant stochastic modeling and multi-objective optimization capabilities provided in the APECS system for process optimization under uncertainty and multiple and sometimes conflicting objectives. The usefulness of these advanced analysis capabilities is illustrated using a simulation and multi-objective optimization of an advanced coal-fired, gasification-based, zero-emissions electricity and hydrogen generation facility with carbon capture.

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1. Introduction

The U.S. Department of Energy (DOE) is investing heavily in Fossil Energy R&D programs to promote the development of advanced power generation systems that meet the Nation's energy needs while achieving a sustainable balance between economic, environmental, and social performance. To achieve performance targets and at the same time reduce the number of costly pilot-scale and demonstration facilities, the designers of these systems increasingly rely on high-fidelity process simulation tools to design and evaluate virtual plants. Developed by the DOE's National Energy Technology Laboratory (NETL), the Advanced Process Engineering Co-Simulator (APECS) is a virtual plant simulator that combines process simulation, equipment simulation, immersive and interactive plant walk-through virtual engineering, and advanced analysis capabilities (Zitney, 2005, 2006a; Zitney et al., 2006). The APECS system uses commercial process simulation software (e.g., Aspen Plus\(^\text{®}\) and equipment modeling software (e.g., FLUENT\(^\text{®}\) computational fluid dynamics) integrated with the process-industry CAPE-OPEN (CO) software standard (Braunschweig & Gani, 2002; Zitney, 2006b) (www.colan.org). APECS provides easy-to-use configuration wizards for use with CO-compliant equipment models including computational fluid dynamics (CFD) models, custom engineering models (CEMs), and reduced-order models (ROMs). CFD models provide a detailed and accurate representation of complex thermal and fluid flow phenomena occurring within a wide variety of power plant equipment items, such as combustors, gasifiers, syngas coolers, carbon capture devices, steam and gas turbines, heat recovery steam generators, cooling towers, and fuel cells. Plug-and-play interoperability of analysis tools in APECS is also facilitated by the use of the CO standard.

For details please refer to a recent paper (Zitney, 2010) describing APECS software capabilities. This work presents a CO-compliant stochastic modeling and multi-objective optimization framework for APECS. This framework enables optimizing model complexities in the face of uncertainty and multiple and sometimes conflicting objectives of design. It also provides a decision support tool to address some of the key questions facing designers and planners of advanced process engineering systems, such as:

- How can different objectives, which are not translated into dollars, be compared and analyzed?
- How does one formulate objectives when there is lack of or inaccurate data and modeling phenomena is not well understood?
- Which objectives are synergistic and which are conflicting, and how does one quantify the trade-offs involved?
- How does one design and operate process plants to be robust, reliable, environmentally friendly, efficient, and cost effective in the face uncertainties?
- What is the probability or risk that a technology will not achieve its expected performance and cost targets?
- How much more will it cost to make the plant more flexible for future considerations?
- How can targeted R&D best reduce critical uncertainties?
The remainder of the paper is arranged as follows. Section 2 describes the theory behind the stochastic modeling capability and the salient features of the stochastic modeling capability. The sampling approach and algorithm for multi-objective optimization are outlined in Section 3 along with the features of multi-objective optimization as implemented in APECs. Section 4 describes an illustrative case study of a next-generation gasification-based power and hydrogen production plant with carbon capture. This section is followed by summary and conclusions in Section 5.

2. Stochastic modeling and efficient sampling techniques

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 computational framework used for simulation of a specified flowsheet. An important shortcoming of these models is their inability to analyze uncertainties rigorously. Uncertainty analysis 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.

Uncertainty analysis consists of four main steps: (1) characterization and quantification of uncertainty in terms of probability distributions, (2) sampling from these distributions, (3) propagation through the modeling framework, (4) analysis of results (Diwekar, Rubin, & Frey, 1997). The first step is of foremost importance and the one on which the validity of the uncertainty analysis is contingent. Characterization refers to the process of representing uncertainty through mathematical expressions in order to facilitate analysis with mathematical tools (Subramanyan, Diwekar, & Goyal, 2004).

2.1. Overview of probability distribution functions

The diverse nature of uncertainty, such as contamination risk, demand and population density uncertainties, and process variations, can be specified in terms of probability distributions. The type of distribution chosen for an uncertain variable reflects the amount of information that is available. It is easier to assume the upper and lower bound of uncertain variables and hence uniform distribution is the first step towards uncertainty quantification. If one can identify the most likely value then triangular distributions can be used. If more data is available then specific properties of distributions are used for characterization. For example, the uniform and log-uniform distributions represent an equal likelihood of a value lying anywhere within a specified range, on either a linear or logarithmic scale, respectively. Further, a normal (Gaussian) distribution reflects a symmetric but varying probability of a parameter value being above or below the mean value. In contrast, lognormal and some triangular distributions are skewed such that there is a higher probability of values lying on one side of the median than the other. In this work, we provide 17 probability distributions to cover the whole range of uncertainties that may arise in process and energy applications.

2.2. Overview of sampling techniques

The stochastic modeling capability offers six sampling techniques (Knuth, 1973). These are:

(1) Monte Carlo sampling (MCS);
(2) Latin hypercube sampling (LHS);
(3) Hammersley sequence sampling (HSS);
(4) Latin hypercube Hammersley sampling (LHHS);
(5) Leaped HSS and
(6) Leaped LHHS.

The following paragraphs explain each sampling technique in more detail.

2.2.1. Monte Carlo sampling

One of the most widely used techniques for sampling from a probability distribution is the Monte Carlo sampling technique, which is based on a pseudo-random generator used to approximate a uniform distribution (i.e., having equal probability in the range from 0 to 1). The specific values for each input variable are selected by inverse transformation over the cumulative probability distribution. A Monte Carlo sampling technique also has the important property that the successive points in the sample are independent.

2.2.2. Latin hypercube sampling

The main advantage of the Monte Carlo method lies in the fact that the results from any Monte Carlo simulation can be treated using classical statistical methods; thus results can be presented in the form of histograms, and methods of statistical estimation and inference are applicable. Nevertheless, in most applications, the actual relationship between successive points in a sample has no physical significance; hence the randomness/independence for approximating a uniform distribution is not critical (Knuth, 1973). Moreover, the error of approximating a distribution by a finite sample depends on the equidistribution properties of the sample used for U(0,1) rather than its randomness. Once it is apparent that the uniformity properties are central to the design of sampling techniques, constrained or stratified sampling techniques become appealing (Morgan & Henrion, 1990). Latin hypercube sampling is one form of stratified sampling that can yield more precise estimates of the distribution function. In latin hypercube sampling, the range of each uncertain parameter X is sub-divided into non-overlapping intervals of equal probability. Fig. 1 shows the stratification scheme (intervals of equal probabilities) for a normal random variable. One value from each interval is selected at random with respect to the probability distribution in the interval. The ‘n’ values thus obtained for X is paired in a random manner (i.e., equally likely combinations) with ‘n’ values of X2. These ‘n’ values are then combined with n values of X3 to form n-triplets, and so on, until n k-tuplets are formed. In median Latin Hypercube (MLHS) this value is chosen as the mid-point of the interval. MLHS is similar to the descriptive sampling described by Saliby (1990).
better uniformity properties compared to other techniques. The main reason for this is that the Hammersley points are an optimal design for placing \( n \) points on a \( k \)-dimensional hypercube. In contrast, other stratified techniques such as the latin hypercube are designed for uniformity along a single dimension and then randomly paired for placement on a \( k \)-dimensional cube. Therefore, the likelihood of such schemes providing good uniformity properties on high dimensional spaces is extremely small. One of the main advantages of Monte Carlo methods is that the number of samples required to obtain a given accuracy of estimates does not scale exponentially with the number of uncertain variables. HSS preserves this property of Monte Carlo. For correlated samples, the approach described by Wang, Diwekar, and Gregoire-Padro (2004), uses rank correlations to preserve the stratified design along each dimension. Although this approach preserves the uniformity properties of the stratified schemes, the optimal location of the Hammersley points are perturbed by imposing the correlation structure. Although the original HSS technique designs start at the same initial point, it can be randomized by choosing the first prime number randomly.

The HSS technique is at least \( 3–100 \) times faster than LHS and Monte Carlo techniques and hence is a preferred technique for uncertainty analysis as well as optimization under uncertainty.

2.2.4. latin hypercube Hammersley sampling

In this sampling technique, we have used the \( k \)-dimensional uniformity of HSS and one dimensional uniformity of LHS to obtain a new sampling technique called Latin hypercube Hammersley sampling (Wang et al., 2004).

In the process of generating samples with LHHS, the sample values of each input variable are first generated using LHS. The next step is to pair them and combine the input vectors. The conventional method is to pair all of them randomly. However, the sample correlation matrix of input variables generated by either LHS or MCS with random pairing processes is not exactly equal to \( I \) and it also shows bad uniformity. Hence restricted pairing procedure is used in all cases. Even when the input variables are independent, the restricted pairing procedure is still employed for the desired correlation matrix \( C \) to make sure there is no actual dependence among the input variables (Diwekar, 2003a; Diwekar & Kalagnanam, 1996, 1997), already showed that Hammersley sequence points have better multidimensional uniformity. In order to characterize the new sampling technique this property, the HSS matrix \( H(N \times k) \) corresponding to van der Waerden scores matrix in Iman and Conover’s approach in LHS, is used in pairing procedures. To avoid the problem associated with \( H(N \times k) \) not having a
correlation matrix equal to I, the sample correlation matrix \( \hat{R}(k \times k) \) 
associated with \( \hat{H}(N \times k) \) is used to find a matrix \( \hat{S} \) so that

\[ \hat{S} \hat{Q}^T = \hat{R} \]

Therefore, the solution of \( \hat{S} \) can be found, which is given by

\[ \hat{S} = \hat{P} \hat{Q}^{-1} \]

and correspondingly the transformation factor for the rank matrix is changed to \( \hat{S} \) and the rank matrix becomes \( \hat{H}^* = H \hat{S}^T \). The correlation matrix of \( \hat{H}^* \) is exactly equal to the desired correlation matrix \( \hat{C} \). The sample can therefore be paired according to the new rank matrix \( \hat{H}^* \) rather than \( H \). In this pairing process, when a correlation structure is not specified, variance of inflation factor (VIF), defined as the largest element on the diagonal of the inverse of the correlation matrix, is computed to detect the large pairing correlations. As the VIF gets much larger than 1, there may be some undesirably large pairing correlations. For VIF > 10, there can be serious collinearity (Marquardt, 1970; Marquardt & Snee, 1975).

Fig. 3 demonstrates the uniformity properties of LHHS. It has been found that the performance of LHHS is most of the time better than HSS. However, unlike MCS or HSS, the performance measure for LHHS is not independent of number of variables or type of functionality used to compute the output distributions.

2.2.5. Leaped HSS and leaped LHHS

It has been recently found that the uniformity property of HSS for higher dimensions (more than 30 uncertain variables) gets distorted as shown in Fig. 4 for the 39-th and 40-th dimension. HSS (and LHSS) is generated based on prime numbers as bases. In order to break this distortion, we introduced primes in prime numbers for higher dimensions. This leaped HSS and LHHS showed better uniformity than the basic HSS and LHHS. For simplicity, we have Leaped HSS and LHHS as a part of the HSS and LHHS techniques in the stochastic modeling capability. When the number of uncertain variables exceeds 30, the switch occurs automatically.

The final step in stochastic simulation process is the propagation of the sampled variables through the model and collecting output distributions for analysis.

2.3. The CAPE-OPEN stochastic simulation capability

The stochastic simulation tool which has been developed using CAPE-OPEN unit operation capability can be used to successfully evaluate different risk and uncertainty scenarios arising in process design and operation. Currently, ASPEN has a case study block to carry out sensitivity analysis, however, it is not possible to systematically vary more than one parameter at given time. This new tool allows uncertainties to be represented by probability distributions, and systematically sample the distributions to generate samples which can be propagated through the flowsheet. The stochastic modeling capability is added to APECS as a unit operation block. The input and output streams to this block are dummy streams and need not be connected to anything in the flowsheet. In the sequence the block should be put first.

Once the stochastic simulation capability is installed and the CO library loaded into the process simulator, the CO-compliant unit operation 'Stochasim' appears as a model icon in the model palette as shown in Fig. 5.
The inputs to stochastic block could be only given through GUI, otherwise there are text files which need to be modified. Once this block is activated, input window shown in Fig. 6 will appear. After completing input for this interface, the user selects the probability distribution specification for each of the uncertain variables as shown in Fig. 7. For each probability distribution, input parameter window or windows appear depending on the distribution. At the end of all distributions, the OK button will be activated to go to the last window.

The final step in the stochastic simulation process is the propagation of the sampled variable through the model by using a stochastic simulation framework flowchart shown in the last input window (Fig. 8). This involves:

1. Reading the generated samples. This is done using the STO-BEG calculator block.
2. Mapping uncertain variables to flowsheet variables. This is done through the block STO-INIT calculator block.
3. Running the flowsheet “Nsamp” times using new sample each time. This is achieved by using the sensitivity block STO-SEN. In this block output parameters of interest are collected.
4. The final analysis is done using STO-ANNL block.

Fig. 8 shows these blocks automatically created by the stochastic simulation capabilities, along with their functionality and calculation sequence using a flowchart. At this stage, an Aspen Plus input file named “Stocha.bkp” containing the three calculator blocks and the sensitivity analysis block necessary for the stochastic simulation process is automatically created when the user clicks on “Proceed to import”. The user can either modify initial input data, for example the number of uncertain parameters, by clicking on “Modify initial data” button or modify the parameters for existing distribution by clicking on “Change parameters for existing distribution”. It should be remembered that these blocks are specific to the ASPEN Plus simulator. Similarly the variables present in flowsheets modeled in other simulators can access the stochastic block information and supply it to the flowsheet. However, since we do not have access to all other simulators, we have discussed the capability in the context of APECS simulator environment.

The output of a stochastic simulation is not a single value of the output variable but a series of values which can be used to construct the cumulative density function (CDF) for the particular output variable. The stochastic block can also provide the sensitivity analysis information for the outputs in terms of the following correlation coefficients.

- PCC: partial correlation coefficient
- SRC: standardized regression coefficient
- PRCC: partial rank correlation coefficient
- SRRC: standardized rank regression coefficient

3. An efficient sampling approach to multi-objective optimization

Multi-objective problems appear in virtually every field and in a wide variety of contexts. The importance of multi-objective optimization can be seen by the large number of applications presented in the literature. The problems solved vary from designing spacecrafts (Sobol, 1992), aircraft control systems (Schy & Giesy, 1988), bridges (Ohtkubo, Dissanayake, & Taniwaki, 1998), vehicles (Starkey, Gray, & Watts, 1988), and highly accurate focusing systems (Eschenauer, 1988), to forecasting manpower supplies (Silverman, Steuer, & Whisman, 1988), selecting portfolios (Tamiz & Jones, 1996), blending sausages (Olson, 1993), planning manufacturing systems (Kumar, Singh, & Tewari, 1991), managing nuclear waste disposal and storage (Diwekar, 2003b; NWTRB, 1996) allocating water resources (Agrell, Lence, & Stam, 1998; Ferreira & Machado, 1996; Wood, Greis, & Steuer, 1982), solving pollution control and management problems (Cohon & Rothley, 1997; Cohon, Scavone, & Solanki, 1988; Fu & Diwekar, 2003; Fu, Diwekar, Young, & Cabezas, 2000) and designing advanced power systems (Subramanyan, Diwekar, & Goyal, 2004). Most of these applications are multi-objective problems of nonlinear nature, which is why we need tools for nonlinear programming capable of handling multiple conflicting or incommensurable (e.g. different units) objectives.

3.1. Multi-objective optimization and pareto set

A generalized multi-objective optimization problem is of the form:

\[ \text{Minimize : } \quad f_i(x), \quad i = 1, \ldots, k, k \geq 2 \]

\[ \text{Subject to : } \quad h_i(x) = 0, \quad i \geq 0 \]

\[ g_j(x) \leq 0, \quad j \geq 0 \]

\[ l_j \leq x_j \leq u_j, \quad j = 1, \ldots, n. \]

The problem under consideration involves a set of \( n \) decision variables represented by the vector \( x = (x_1, x_2, \ldots, x_n) \). The equality constraints \( h_i(x), i \geq 0: \mathbb{R}^n \rightarrow \mathbb{R} \), and inequality constraints \( g_j(x) \leq 0, j \geq 0: \mathbb{R}^n \rightarrow \mathbb{R} \) are real-valued (possibly nonlinear) constraint functions, and \( l_j \) and \( u_j \) are given lower and upper bounds of
decision variable $x_j$ (allowed to be $-\infty$ and/or $+\infty$). Both the equality constraints $h_i(x)$ and inequality constraints $g_j(x)$ are assumed to be continuously differentiable and the feasible decision region $S$ defined by (1) is assumed to be a nonempty subset of $\mathbb{R}^n$. If $f=0$ and $j=0$, the problem becomes unconstrained. The decision situation involves $k(\geq 2)$ continuously differentiable nonlinear objective functions $f_j: \mathbb{R}^n \rightarrow \mathbb{R}$. The vector of objective functions is $f(x) = (f_1(x), f_2(x), \ldots, f_k(x))^T$ or $z = (z_1, \ldots, z_k)^T$, where $z_i = f_i(x)$ for all $i = 1, \ldots, k$ and the feasible objective region $Z$ defined by (1) is assumed to be a nonempty subset of $\mathbb{R}^k$. Without loss of generality, we assume that all the objective functions are to be minimized simultaneously (note that an objective of the maximization type could be converted to one of the minimization type by multiplying the objective function by $-1$).

The solution of a multi-objective optimization problem is a set of solution alternatives called the Pareto set. For each of these solution alternatives, it is impossible to improve one objective without sacrificing the value of another relative to some other solution alternatives in the set. A more formal definition of Pareto optimality is the following:

A decision vector $\bar{x} \in S$ is Pareto optimal (also called Edgeworth–Pareto optimal, the efficient solution, the nondominated, the functional efficient) for problem (1) if there does not exist another decision vector $\bar{x} \in S$ such that $f_i(\bar{x}) \leq f_i(\bar{x})^*$ for all $i = 1, \ldots, k$ and $f_j(\bar{x}) < f_j(\bar{x})^*$ for at least one index $j$.

An objective vector $\bar{z} \in Z$ is Pareto optimal if there does not exist another objective vector $z \in Z$ such that $z_i \geq z_i^*$ for all $i = 1, \ldots, k$ and $z_j < z_j^*$ for at least one index $j$; or equivalently, $\bar{z}$ is Pareto optimal if the decision vector corresponding to it is Pareto optimal.

There are usually many (infinite in number) Pareto optimal solutions. The collection of these is called the Pareto set. The result of the application of a nonlinear multi-objective technique to a decision problem is the Pareto set for the problem, and it is from this subset of potential solutions that the final, preferred decision is chosen by the decision-makers.

3.2. Pareto set generating methods

There is a large array of analytical techniques for multi-objective optimization problems. In general, the multi-objective optimization methods are divided into two basic types: preference-based methods and generating methods (Diwekar, 2003b). Here we are concentrating on the generating method. Generating methods provide a great deal of information, emphasizing the Pareto optimal set or the range of choice available to decision-makers, and providing the trade-off information of one objective versus another. Generating techniques can be further divided into two sub-classes: no-preference methods and a posteriori methods. A Priori methods, such as weighting methods and constraint methods, can obtain each point of the Pareto set. The idea of the weighting methods (Gass & Saaty, 1955; Zadeh, 1963) is to associate each objective function $f_i(x)$ with a weighting coefficient $w_i \geq 0$ and minimize the weighted sum of the objectives. In this way, the multi-objective optimization problem is transformed into a series of single objective optimization problems. The Pareto set can be derived by solving a large number of single objective optimization problems, which are created by modifying the weighting factors of the objectives. However, there are three major disadvantages of using the weighting method. (a) Its inefficiency that arises due to
the linear combination of objectives. (b) Its difficulty to control the region of the nondominated surface on which the decision-maker is heavily favored. For example, a small change in the weighting coefficients may cause large changes in the objective vectors, and dramatically different weighting coefficients may produce nearly similar objective vectors. In addition, an evenly distributed set of weighting vectors does not necessarily produce an evenly distributed representation of the Pareto set, even if the problem is convex (Das & Dennis, 1998). (c) Its lack of robustness. For example, all of the Pareto optimal points cannot be found if the problem is non-convex.

The constraint methods (Cohon, 1978; Diwekar, 2003b; Haines, Lasdon, & Wismer, 1971; Zeleny, 1982) belong to another type of posterior methods for generating the Pareto set. The basic strategy is also to transform the multi-objective optimization problem into a series of single objective optimization problems. The idea is to pick one of the objectives to minimize (say \(Z_i\)) while each of the others \((Z_j, i = 1, \ldots, k, i \neq j)\) is turned into an inequality constraint with parametric right-hand sides \((\varepsilon_i, i = 1, \ldots, k, i \neq j)\). The problem takes the form:

Minimize :

\[
Z_l = f_l(\bar{x})
\]

Subject to :

\[
Z_i = f_i(\bar{x}) \leq \varepsilon_i, \quad i = 1, \ldots, k, i \neq l
\]

\[
h_l(\bar{x}) = 0, \quad j > 0
\]

\[
g_j(\bar{x}) \leq 0, \quad j > 0
\]

\[
\bar{x} = (x_1, \ldots, x_n)
\]

Solving repeatedly for different values of \(\varepsilon_1, \ldots, \varepsilon_{l-1}, \varepsilon_{l+1}, \ldots, \varepsilon_k\) leads to the Pareto set. This method also needs to obtain solutions for a large number of single objective optimization problems. The computational burden of the constraint methods is more laborious than the weighting methods for finding each Pareto solution because the number of constraints is larger than that of the weighting method, and sometimes no feasible solution can be found for some particular combinations of the right-hand sides. In reality, the influence is assumed to be trivial since there are often a much larger number of original constraints than the number of objectives in large-scale real-world applications. Furthermore, the constraint method offers the advantages of better control over exploration of the Pareto set and of being able to locate points anywhere along the Pareto surface. Theoretically, every Pareto optimal solution of any multi-objective optimization problem can be found by the constraint method through altering the upper bounds and the function to be minimized. Therefore, the constraint method is a relatively more robust method than the weighting method and a new and efficient multi-objective optimization algorithm based on the Hammersley sequence sampling technique (Diwekar & Kalagnanam, 1997); rooted in the constraint method to solve large-scale real-world problems is presented below (Fu & Diwekar, 2004).

3.3. MINSOOP: a new nonlinear multi-objective optimization algorithm

The new algorithm called minimization of single objective optimization problems (MINSOOP) is based on the assumption that the problem is equivalent to the results of calculating an integral over the space of objectives. Consider the approximation of an integral of a \((k − 1)\)-dimensional (with a \(k\)-objective problem) continuous function by sampling its values at a finite set of points. One straightforward approach is to place the points along equally spaced intervals on a \((k − 1)\)-dimensional grid, which represents the traditional constraint method. Although this is a good arrangement, the number of points required increases rapidly as the number of objectives increases. For example, if there are six objectives and five of them are evaluated over 10 points for each objective, we would have to solve 100,000 optimization problems. Alternatively, one can use a Monte Carlo sampling (MCS) technique, where the points are chosen randomly. The approximation of the integral is then based on the function evaluation at these points. On average, however, the error of approximation (from central limit theorem) is of the order \(O(N^{−1/2})\), which also means the number of points \((N)\) required to keep the error within \(\varepsilon\) is bound by \(1/\varepsilon^2\) (NWTRB, 1996). The remarkable feature is that the bound is not dependent on the dimension \((k − 1)\) in this case. This means MCS methods are unlikely to scale exponentially with increasing objective functions. However, MCS methods are based on pseudo-random number generators, and do not have good uniformity.

The new multi-objective optimization algorithm uses the HSS technique to generate combinations of the right-hand sides \(\varepsilon_i, (i = 1, \ldots, k, i \neq l)\) of the traditional constraint method. The steps for a multi-objective problem with \(k\) objectives (to be minimized) are listed as follows:

Step 1. Solve \(k\) single objective optimization problems individually with the original constraints of a multi-objective problem to find the optimal solution for each of the individual \(k\) objectives.

Step 2. Compute the value of each of the \(k\) objectives at each of the \(k\) individual optimal solutions. In this way, an approximation of the potential range of values for each of the \(k\) objectives is determined and saved in a table (called payoff table). The minimum possible value is the individual optimal (minimizing) solution. The approximate maximum possible value of the Pareto set is the maximum value for that objective found when minimizing the other \(k − 1\) objectives individually.

Step 3. Select a single objective (e.g. \(Z_i\)) to be minimized. Transform the remaining \(k − 1\) objectives into inequality constraints of the form \(Z_j \leq \varepsilon_j, (i = 1, \ldots, k, i \neq l)\) and add these new \(k − 1\) constraints to the original set of constraints. Then the original multi-objective optimization problem is transformed into a family of single objective optimization problems with parametric right-hand sides.

Step 4. Select a desired number of single objective optimization problems to be solved to represent the Pareto set. Using the HSS technique to generate the desired number of combinations of the inequality constraint values \(\varepsilon_1, \ldots, \varepsilon_{l-1}, \varepsilon_{l+1}, \ldots, \varepsilon_k\) within the range determined in Step 2.

Step 5. Solve the constrained problems set up in Step 4 for every combination of the right-hand-side values determined in Step 3. These feasible solutions form an approximation for the Pareto set.

Fig. 9 shows the number of nonlinear sub-problems solved in an approximate Pareto surface versus the number of objectives using the same accuracy for both methods (e.g. 99.9% of the mean and 99% of the variance). Results show that the number of nonlinear sub-problems to be solved for the fixed accuracy increases rapidly as the number of objective functions increases for the traditional constraint method. However, there is no significant increase for the new algorithm as the number of objectives increases. This indicates that the computational savings by using the new nonlinear multi-objective optimization algorithm increases dramatically as the number of objectives increases, as shown in Fig. 9. This result is particularly important, as the computational burden for a large number of objectives is often extreme for all other multi-objective procedures. This indicates a breakthrough for solving high-dimensional problems.

To make this algorithm more accessible to APECs users, we have created an easy-to-use tool which simplifies and automates the process of setting up and solving a multi-objective optimization. Developed using Visual Basic 6.0 and FORTRAN, the tool is a CO-compliant unit operation model, ‘MOPsim’. When this block is put in the flowsheet, the GUI opens with Fig. 10, where the user can
specify the inputs for the multi-objective optimization including the number of objectives, number of decision variables, number of inequality constraints, and the number of equality constraints. The last input is “Number of samples for parametric RHS” and corresponds to how many points in the Pareto set (trade-off surface) the user wants to obtain. As shown in Fig. 10, the MOPsim tool then prompts the user and provides a list box to specify which objective has to be maximized and which one has to be minimized. Upon completing specification of “Min” or “Max” for each objective, the user clicks on the “Proceed” button to display the final information window as shown in Fig. 11. This dialog shows shows the multi-objective optimization features, calculation sequence, and subsequent steps to be completed. An Aspen Plus file named “MOP.bkp” containing the blocks necessary for the multi-objective optimization is created automatically. Similar information transfer can be done with other simulators also. The final results are found in the file “MOPRES.dat” in the current working directory. Final results provide the Pareto or the trade-off

![Fig. 9. Comparison of MINSOOP with traditional constraint method.](image-url)

![Fig. 10. Input specification for multi-objective optimization capability.](image-url)

![Fig. 11. Multi-objective optimization block calculation sequence and functionality.](image-url)
surfaces for all the objectives in terms of optimal objectives and optimal decision variables. The first approximation of the Pareto surface is the payoff table.

4. Illustrative case study

This section describes the advanced gasification-based power and hydrogen coproduction case study and illustrates the application of the stochastic analysis and multi-objective optimization tools.

4.1. Power and hydrogen coproduction plant with carbon capture

An advanced coal-fired, gasification-based power and hydrogen coproduction plant with carbon capture (Rao, Samuelson, & Robson, 2003; Rao, Samuelson, Robson, Washom, & Berenyi, 2006) is used here as a case study. The ground coal along with ground limestone for in-bed sulfur capture is added to the upper stage of the mixing zone of an advanced transport reactor (ATR) gasifier. The syngas, mainly H₂ and carbon monoxide (CO), leaving the gasifier is cooled to a low temperature by generating superheating steam to stay within the temperature limits of commercially available high temperature sweet shift catalysts. A fraction of the syngas is utilized as transport gas for feeding the solids to the ATR. The remainder of the syngas is cleaned and then combined with intermediate pressure (IP) steam. This mixture is fed to the shift/membrane unit to form additional H₂ and to separate the H₂. The recovered H₂ along with some additional H₂ recovered downstream of the fuel cell is cooled and compressed to pipeline for export. The tail gas from the membrane unit consisting primarily of CO, carbon dioxide (CO₂), a portion of H₂ that is not recovered, water and inerts such as nitrogen are fed to a fixed bed reactor containing a methanation catalyst followed by a turbo-expander. The methanation/shift reactions serve to (1) producing additional methane (2) raising the temperature of the syngas. The increased methane content of the syngas assists of providing a heat sink for the heat generated within solid oxide fuel cells (SOFC) while the increased temperature of the syngas increases the power developed by the turbo-expander. The methanated/expanded syngas is fed to the anode side of the cells. Compressed air supplied by the gas turbine is heated in a regenerator and then supplied to the cathode side of the cells. The anode exhaust gas after heat recovery is fed to a second shift unit where additional H₂ is formed by shifting the remaining CO. The H₂ in the shifted gas is captured and exported to pipeline. The non-permeate is fed to a catalytic combustor using O₂ from the ion transport membrane (ITM) or oxygen transport membrane (OTM) unit to fully remove the small amounts of any remaining CO and H₂. This stream is cooled and pressurized for storage. The hot air exiting the SOFC is preheated and fed to ITM/OTM unit. The oxygen exits from the ITM/OTM unit at atmospheric pressure and is recycled back the gasifier. The non-permeate from the ITM/OTM is expanded in gas turbine and exhausts to a Heat Recovery Steam Generator (HRSG) unit for heat recovery.

The process schematic of the power and hydrogen coproduction plant is shown in Fig. 12. Table 1 summarizes the Aspen Plus steady-state simulation results for plant performance including power production, efficiency, and CO₂ emissions. We assumed here internal power consumption to be fixed at 45.4 MW, as specified in Rao et al. (2003, 2006).


4.2. Uncertainty analysis of the coproduction plant

The advanced gasification-based coproduction plant is a fairly new and futuristic design and hence the system level models used
for predicting the performance for the fuel cells and other modules like the gasifier have significant uncertainties in them (Rao et al., 2003, 2006). Therefore, we have considered two sources of uncertainties in this design:

- Uncertainties in the SOFC current density characteristics.
- Uncertainties in the gasifier temperature.

In case of the SOFC, an uncertainty factor (UF) defined as the ratio of the model predicted voltage to the experimental voltage for each current density, is introduced to characterize uncertainty. The next step is uncertainty quantification, which refers to the representation of uncertainty with probability distribution functions (PDF) illustrating the frequency of occurrence of each uncertainty. Figs. 13 and 14 illustrate the uncertainty quantification for the SOFC and gasifier units respectively. Due to the lack of experimental data for the ATR gasifier used in this design, we assume a 5% normal variation around the design temperature (1052 °C).

After uncertainty quantification, the next step is to sample the distribution and propagate the uncertainties through the model. We have used the efficient Hammersley sequence sampling (HSS). The samples are propagated through the process model using the stochastic framework.

The cumulative distribution functions (CDF) of current density, CO₂ emission, and overall thermal efficiency are plotted in Figs. 15–17, respectively and compared to the outcome of deterministic case. The deterministic case value is represented by a straight line. In Fig. 15, there is only a 10% probability of current density being equal to the deterministic value. There is a 90% chance that the SOFC current density is higher than that predicted by the base case. This result reinforces the need for uncertainty analysis of this design. In Fig. 16, there is a 40% chance of the CO₂ emissions being equal to the deterministic value. This is certainly better than that of the SOFC current density, but the probability is still on the lesser side. In Fig. 17, there is a 60% chance that the overall efficiency is equal to that predicted by the base case which is better than the previous two output variables. Thus considering the deterministic case alone is not sufficient. The incorporation of uncertainties is important for accurate estimation.
4.3. Multi-objective optimization of the coproduction plant

The main objectives to be optimized for this process are:

1. Overall efficiency of the process
2. CO\(_2\) emissions (kg/kWh)
3. SOFC current density (mA/cm\(^2\)), CDS

The first task is to perform a sensitivity analysis to identify the design and input variables which have the maximum impact on the selected objectives. For this purpose a sampling approach based on partial rank correlation coefficients (PRCC) is used. Please note that PRCC analysis can be done with the stochastic simulation tool described in Section 2. The partial correlation coefficients calculated on ranks are a good measure of the strength of monotonic relations between inputs and outputs, whether linear or not (Morgan & Henrion, 1990), and provide sensitivity for the whole range unlike partial derivatives normally used in this analysis. Input variables with higher PRCC have stronger input relationship. The nine design variables initially chosen for the analysis included:

1. Operating temperature of gasifier
2. Inlet coal mass flowrate
3. Operating temperature of SOFC module
4. Operating pressure of SOFC module
5. SOFC fuel utilization
6. Temperature of shift reactor module
7. Conversion of reaction #1 in stoichiometric reactor module,
8. Conversion of reaction #2 in stoichiometric reactor module,

The results of the sensitivity analysis are shown in Table 2. The top three variables were chosen for the final MOP framework based on their PRCC values. The final decision variables were:

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<thead>
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<th>Table 2</th>
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<td>PRCC sensitivity analysis results.</td>
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<td>Design variable</td>
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1. SOFC fuel utilization
2. Inlet rate of drycoal (kg/h)
3. Operating temperature of the SOFC (K)

The final MOP problem formulation is given by:

Objectives:

- Min CO\(_2\) emissions
- Max current density SOFC
- Max overall efficiency

Subject to

- Mass and energy balance constraints
- Power rating of 475.5 MW (base case)

Decision variables

- Fuel utilization in SOFC
- Inlet rate of dry coal
- Temperature of the SOFC

The approach here is to define the pre-defined objective names as parameter variables in the “Define” sheet and the assignment of these objective variables is taken care of by the pre-defined calculator blocks created automatically by the multi-objective optimization tool.

5. Results and analysis

Table 3 shows the payoff table for the advanced power and hydrogen coproduction plant. As mentioned above, the payoff is a first approximation to the complete trade-off surface and gives the maximum and minimum bounds for all the objectives.

Table 3 shows the minimum and maximum bounds for each objective. It should be noted that this is a highly nonlinear process and hence multiple optimum designs cannot be avoided. In Table 3, the maximum SOFC current density (Max CDS) design predicted has a very high overall efficiency because the inlet coal flowrate is the lowest for this design. The opposite is true for the ‘Min CDS’
case where the overall efficiency is low because the inlet flowrate is higher. This is also true for the overall efficiency designs. Also note that the SOFC fuel utilization and the SOFC temperature are the highest for the ‘Max CDS’ design. In the Min CDS design, though the SOFC fuel utilization is high, the temperature has reduced considerably. The overall efficiency and CO2 emissions are inversely proportional to each other. Hence for the Max CO2EM design, the efficiency is lower and vice versa for the Min CO2EM design.

Fig. 18 shows the complete trade-off surface for the three objectives: CO2 emissions in the X-axis, SOFC current density in the Y-axis and the overall efficiency as the contours in the Z-axis. The dominant trend is clearly illustrated by the abundance of regions in the surface corresponding to an overall efficiency range of 0.68–0.70. This region runs over the entire range of SOFC current density and low to moderate values of CO2 emissions. The dark regions are areas of low overall efficiency (0.60–0.62) and as expected these are regions of high CO2 emissions. One interesting point to be noted here is that the lower efficiency areas occur in regions of low to moderate SOFC current density and the regions of higher current density correspond to higher efficiencies. This seems to be an anomaly as more the current is drawn; the lesser should be the efficiency. However, it should be noted that this is a overall cycle efficiency contributed by the SOFC, gas turbine and steam turbine cycles. It should be noted that, in the payoff table, the maximum SOFC current density was computed as 167 mA/cm² while we obtained designs with current densities greater than this value in this Pareto surface. This is because the surface is highly non-convex leading to the existence of multiple local optima. From the plot we can define the preferred operational regions to be the circled region of high current density, low-moderate CO2 emissions and high overall efficiency.

Fig. 19 shows the decision variables corresponding to the trade-off surfaces shown in Fig. 18. In this figure, the SOFC fuel utilization values are plotted on the Y-axis, inlet coal flow rate on the X-axis and the overall efficiency as contours on the Z-axis. As the inlet coal flow rate increases, the overall efficiency decreases because the inlet power becomes relatively greater compared to the outlet power. Hence the area on the right-hand side of the plot is corresponding to low efficiencies and high coal inlet flowrate. The highest efficiency is in the left extreme region of the plot corresponding to low inlet flowrates.

One region to be noted in particular is corresponding to relatively higher overall efficiency in the extreme bottom right region of the plot corresponding to the highest inlet coal flow rates and lowest SOFC fuel utilization. The reason for higher efficiencies despite the high inlet coal flow rate could be attributed to the low SOFC fuel utilization and hence lower current density leading to increase in the efficiency.

6. Summary

This paper described the CAPE-OPEN compliant stochastic modeling and multi-objective optimization capability as implemented in NETL’s APECS system. Illustrative case study of an advanced coal-fired gasification-based power and hydrogen plant with carbon capture shows the usefulness of both computational capabilities. Stochastic analysis results provide probabilistic estimates of the outcome. Further, a stochastic model also provides sensitivity analysis information for multi-objective optimization decision variable identification. Apart from this, it provides a reduced order model based multivariate regression. The stochastic analysis tool exploits efficient sampling techniques that are computationally efficient.

The solution of a multi-objective optimization problem is not a single solution but a Pareto surface. To obtain these Pareto surfaces for deterministic and stochastic analysis, we needed an efficient framework. The framework presented here is based on efficient algorithms like the MINSOOP algorithm for multi-objective optimization, and efficient sampling techniques for uncertainty analysis. The pay-off table, a first approximation to Pareto sur-
face, gave an initial indication of similarity between the designs. The algorithm provides trade-off surfaces in objective as well as decision variable space. The stochastic analysis and multi-objective optimization capabilities in APECS provide process optimization in the face of uncertainty and multiple and sometimes conflicting objectives. Such advanced process systems engineering capabilities will help reduce the time, cost, and technical risk in realizing high-efficiency, zero-emission gasification-based power plants.

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References


