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Parameter Design Methodology for Chemical Processes Using a Simulator

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Parameter design is a method popularized by the Japanese quality expert G. Taguchi, for designing products and manufacturing processes that are robust in the face of uncontrollable variations. At the design stage, the goal of parameter design is to identify design settings that make the product performance less sensitive to the effects of manufacturing and environmental variations and deterioration. Because parameter design reduces performance variation by reducing the influence of the sources of variation rather than by controlling them, it is a cost-effective technique for improving quality. A recent study on the application of parameter design methodology for chemical processes reported that the use of Taguchi's method was not justified and a method based on Monte Carlo simulation combined with optimization was shown to be more effective. However, this method is computationally intensive as a large number of samples are necessary to achieve the given accuracy. Additionally, determination of the number of sample runs required is based on experimentation due to a lack of systematic sampling methods. In an attempt to overcome these problems, the use of a stochastic modeling capability combined with an optimizer is presented in this paper. The objective is that of providing an effective means for application of parameter design methodologies to chemical processes using the ASPEN simulator. This implementation not only presents a generalized tool for use by chemical engineers at large but also provides systematic estimates of the number of sample runs required to attain the specified accuracy. The stochastic model employs the technique of Latin hypercube sampling instead of the traditional Monte Carlo technique and hence has a great potential to reduce the required number of samples. The methodology is illustrated via an example problem of designing a chemical process.

1. Introduction

When the Ina tile company of Japan found that the uneven temperature profile of its kiln was causing unacceptable variation in tile size, it could have attempted to solve the problem with expensive modification of kilns. Instead, it chose to make an inexpensive change in the settings of the tile design parameters to reduce sensitivity to temperature variation. Using a statistically planned experiment, the company found that increasing lime content of the clay from 1% to 5% reduced the tile size variation by a factor of 10 (Taguchi and Wu, 1980). A technique such as this that reduces the variation by reducing the sensitivity of an engineering design to the sources of variation rather than by controlling them is called *parameter design.*

In order to minimize deviations from product specifications, the usual approach has been to design an automatic control system which keeps the process output specifications on target, despite changes in the process input. In such an approach, the control engineer is often presented with difficult control problems that may require extensive and expensive modifications to both process and control system hardware to obtain satisfactory performance of the control system. Furthermore, the effectiveness of the control system is highly dependent upon the nominal values of the operating variables and the mechanical design which are set by the designer of the processing unit. The high degree of interactions among these design problems is now widely recognized, and current research trends have been aimed at designing the unit and the control system concurrently. A recent article by Sheffield (1992) highlights the importance of such an integrated approach at the design stage which helps to avoid difficult control problems at the end of the line. Parameter design methodology is an off-line quality control method, popularized by Dr. G. Taguchi, for designing products and processes that are robust to uncontrollable variation at the design stage.

Taguchi has outlined a three-step approach to off-line quality control namely, *system design, parameter design,* and *tolerance design. System design* is the process of applying scientific and engineering knowledge to produce a basic functional prototype design. The prototype model defines the initial settings of product or process design.

Parameter design is an investigation conducted to identify settings that minimize (or at least reduce) the performance variation. This is a key step to achieve high quality without increasing the cost.

Tolerance design is the last step and is only employed if the reduced variation obtained through parameter design is not sufficient. It involves tightening tolerances on product parameters or process factors whose variations impart large influence on the output variation.

The rapid growth of interest in the Taguchi approach over the last few years led to a great expansion in the number of published case studies relating to different areas of industrial activities (Bendell et al., 1989). Although the popularity of Taguchi approach seems to be pervasive in all engineering branches, application of this procedure to chemical industries has not been widely reported. Boudriga (1990) presented one of the first systematic studies of using different statistical approaches to the problem of off-line quality control for chemical processes.

Chemical industries are well served in the area of *System design* by process simulators such as FLOWTRAN, PRO/II, CHEMSHARE, and ASPEN. Although these simulators are based on a deterministic framework, a recent work by us on the addition of a generalized stochastic

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modeling capability (Diwekar and Rubin, 1991) around the public version of ASPEN simulator opened up new areas of research and analysis and provided an important tool for design research. This paper presents a methodological approach to parameter design of chemical processes which centers around the ASPEN simulator and is based on the stochastic modeling capability. The paper also analyzes different sampling techniques and provides an insight into the stochastic optimization problem underlying the parameter design methodology. The methodology is discussed and illustrated using an example problem of a chemical process flowsheet.

2. Taguchi Approach to Parameter Design

In parameter design, Taguchi's stated objective is to find settings of the product or process design parameters which minimize an average quadratic loss function defined as the average standard deviation of the response from a target value. In order to select the settings of the design parameters, a set of measures called signal-to-noise ratio (SN) needs to be maximized. Taguchi uses the so-called orthogonal-array designs to arrive at the optimal settings. Recently, several statisticians (Kacker, 1985; Hunter, 1985; Leon et al., 1987) tried to establish the relation between loss function and the SN measure and provided insights into the Taguchi approach which was surrounded by a mystique that few could unveil.

Kacker (1985), in an introduction to the methods of Taguchi, presented the philosophy and terminologies behind the Taguchi approach. In the same article, he explains the concept of orthogonal arrays which are essentially statistical experiments with smaller runs. Both Kacker (1985) and Hunter (1985) suggested that the use of orthogonal arrays could be misleading. Leon et al. (1987) provided the relation between SN ratio and the loss function. They showed that by using the signal-to-noise ratio, a logarithmic transformation was performed on the raw data. The objective of this transformation is to make the mean and the variance independent. However, in many situations this transformation does not eliminate or reduce the coupling of mean and variance. In short, all these studies indicate that the Taguchi approach is very efficient and useful only when the objective function has a quadratic form and no interactions exist between the mean and the variance. Therefore, a functional relationship between the output and input is required *a priori* to decide whether the Taguchi approach should be used or not, and such a relationship may not be available for many real-world problems.

Boudriga (1990) explored different approaches to parameter design for chemical processes and also arrived at the foregoing conclusion. It was stated that for a generalized application of parameter design strategy, Taguchi's approach of using orthogonal arrays to maximize the signal-to-noise ratio is not justified and one has to resort to stochastic optimization techniques. Boudriga used Monte Carlo simulations along with nonlinear optimization techniques to minimize the variance. Boudriga's work on parameter design of chemical processes and the recently developed stochastic modeling capability around a chemical process simulator (Diwekar and Rubin, 1991) forms the basis for a generalized framework for parameter design methodology described in the next section.

3. A Generalized Framework for the Parameter Design of Chemical Processes

The present approach involves adding an optimization capability based on the successive quadratic programming (SQP) technique to the public version of the ASPEN simulator in the form of a unit operation block. The modular nature of both the stochastic modeling and optimization capabilities allowed the development of the generalized framework for a parameter design method around a chemical process simulator. The structure of the framework and its use are briefly described below.

The optimization block provides the stochastic block with the optimal values of the decision variables in terms of the nominal values of the uncertain variables. The deviations in the input variables are expressed in terms of the standard deviation and mean given by

$$E = \frac{\sigma_i 100\%}{\mu_i} \tag{1}$$

where E is the error level, and σ_i and μ_i are, respectively, the standard deviation and the mean value of input variable i. The stochastic block characterizes this information in terms of probability distributions and analyzes their effect on the selected output variables. The stochastic block is linked with the flowsheet on one side and with the optimization block on the other side. This type of stochastic optimization framework can be used for parameter design methodology which involves (1) Identifying the key decision variables, (2) specifying input uncertainties or variabilities in terms of percentage deviations and types of error distribution, (3) specifying the correlation structure of the interdependent parameters, if any, (4) sampling the distributions of the specified parameters in an iterative fashion, (5) propagating the effect of uncertainties through the process flowsheet and collecting the outputs of interest, and (6) solving the following optimization problem.

$$\underset{\mu_j,\, j = 1, \ldots, \mathrm{nv}}{\text{minimize}} \quad \sigma_o^2 = \sum_{i=1}^{N} (y_i - \bar{y})^2 \tag{2}$$

where y_i is the output of the sample i and σ_o^2 is the variance of the output.

The optimization block invokes the stochastic block with the set of nominal values of the parameters. The stochastic block assigns a probability distribution based on the nominal values and the specified error levels. The distributions are selected from the set of eight types of distributions (normal, lognormal, uniform, loguniform, modified uniform, beta, and triangular) available in the stochastic block or from user-defined distributions. Subsequently, it uses either Latin hypercube sampling or random sampling to pass the values of each uncertain input variable to the flowsheet. After the flowsheet simulation is run, the output variables of interest are collected. The stochastic simulation cycle is then repeated for a new set of samples selected from the probabilistic distributions. A fortran block, STCREC, is used to control the cycling of the stochastic block, and another block, called STCTAIL, is used to access and assign samples to the model parameters.

After all the samples or observations have gone through the cycle for a specified number of times, the stochastic block analyzes the output and provides information on the sample variance to the optimization block, either as a single value or in the form of a response surface. A response surface could be used as a crude model to study the influence of several independent variables on the response of dependent variable. The stochastic block has a feature to generate the response surface using step-wise regression and is based on the method outlined by Iman et al. (1981a, b). The information about variance, together

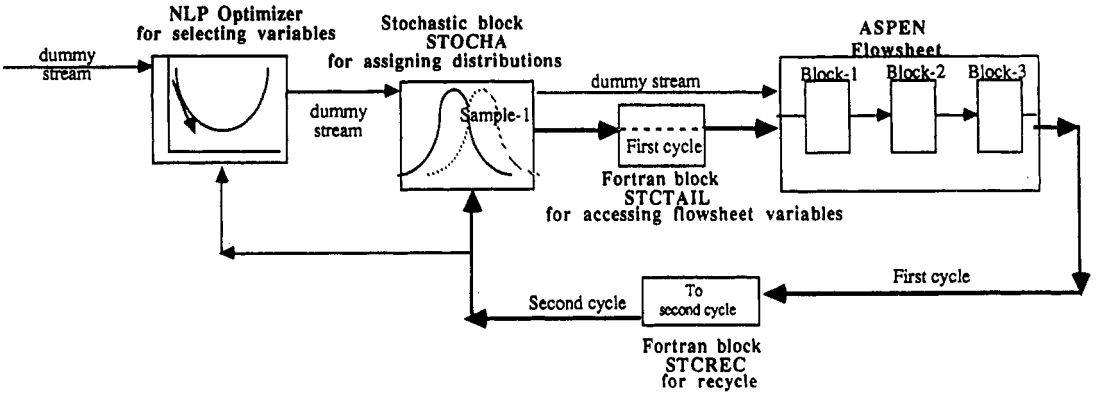


Figure 1. Generalized framework for the parameter design of chemical processes.

with the partial derivatives of the objective function with respect to decision variables, is utilized by the optimization block to update the values of the decision variables. The partial derivatives are calculated by the optimization block by perturbing the values of the decision variables and observing the corresponding changes to the objective function. The iterative sequence is carried out until the optimality conditions are satisfied.

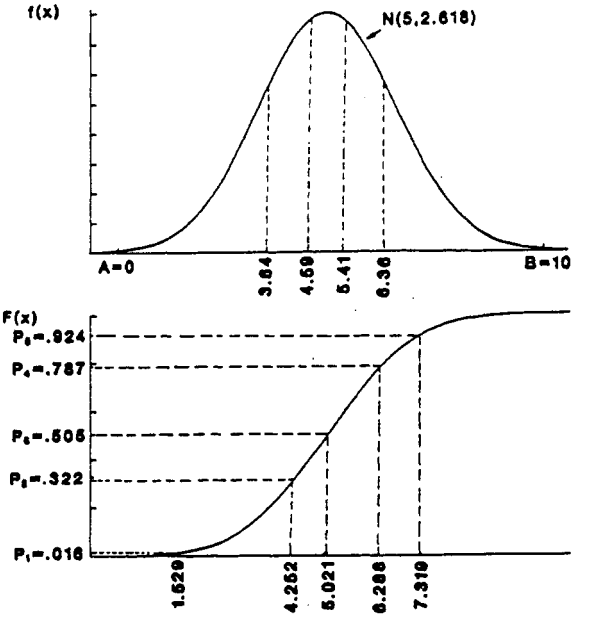
Figure 1 shows the use of the stochastic optimization framework for the parameter design of a chemical process. The cycle for the parameters consists of (a) the optimization block, OPTM, (b) the stochastic block, STOCHA, for assigning parameter uncertainty distributions and passing the information about variance to the optimization block, (c) the Fortran block, STCTAIL, for accessing variables and assigning sampled values, and (d) the Fortran recycle block, STCREC, for data output collection and recycling.

4. Latin Hypercube Sampling and Random Monte Carlo Simulations

There are two sampling methods available within the stochastic unit operations block—random Monte Carlo sampling (MCS) and Latin hypercube sampling (LHS). Although our earlier paper (Diwekar and Rubin, 1991) describes these techniques in brief, it was found essential to discuss these two methods in detail in this paper because the sampling will be used in the context of stochastic optimization where computational efficiency as well as precision plays an important role.

Random Monte Carlo simulation is the well-known and simplest sampling method and is most widely used. In a crude Monte Carlo analysis, a value is drawn at random from the distributions of each input. A sample defined by a set of random values for each input, is used by the model to compute the output values. Boudriga (1990) used the Random Monte Carlo Simulations to compute the variance of the output in the application of the parameter design methodology to their problem. It is often not realized that the primary value of Monte Carlo methods is not the randomness of the sampling but the resulting equidistribution properties of the sets of points in the parameter space. Once this is recognized, the other systematic or stratified sampling techniques become more appealing (Morgan and Henrion, 1990).

In a stratified sampling technique, the sample space for an input parameter is divided into strata, and input values are obtained by sampling separately from each stratum, instead of from the distribution as a whole. Latin hypercube sampling (LHS) represents one class of stratified sampling (Iman and Shortencarier, 1984). In the LHS method, a distribution is divided into N intervals of



Interval m	Random no. R_m	Scaled Probability P_m	Corresponding Observation
1	0.080	0.016	1.529
2	0.610	0.322	4.252
3	0.525	0.505	5.021
4	0.935	0.787	6.288
5	0.620	0.924	7.319

Figure 2. Interval endpoints used with a LHS with size 5 (top) and specific values selected through the inverse of the distribution function (bottom) (Iman and Shortencarier, 1984).

equal probability, where N represents the number of samples, and one sample is taken at random from within each interval. LHS guarantees that the values from the entire range of the distribution are sampled in proportion to the probability density of the distribution.

Figure 2 shows the procedure for selecting five samples using Latin hypercube sampling for a normal distribution. To get the specific values, 5 random numbers are selected between 0 and 1. These numbers (R_m, m = 1, ..., 5) are then scaled to obtain the following probabilities.

$$P_m = R_m(1.0/5) + (m-1)(1.0/5), \quad m = 1, ..., 5 \qquad (3)$$

This ensures that exactly one probability, P_m will fall within each interval as shown on the probability axis. The values of P_m are then used to obtain the inverse of the distribution function to generate the specific values used in LHS (Figure 2). Note that the values generated for each input are in the ascending order of probability. The final step in

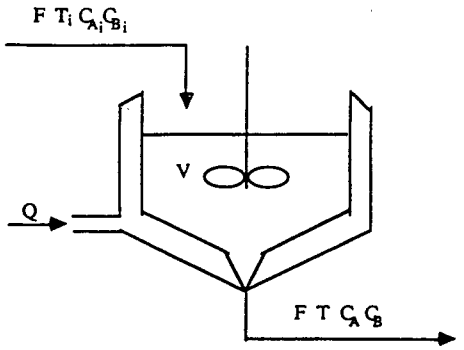


Figure 3. The nonisothermal CSTR.

sampling involves pairing the selected values, done either randomly or using the restricted technique of Iman and Conover (1982), where the user-specified correlations are used.

Since the LHS technique samples the distributions over the entire range of probable values, the number of samples required to adequately represent a distribution is normally much less than that required in Monte Carlo Techniques. However, the number of samples required for an accurate simulation is harder to compute (using statistical analysis) for LHS than for Monte Carlo Simulations.

5. Sampling Accuracy

Before starting the stochastic optimization runs, the accuracy of the sampling process is evaluated. The example of a continuous stirred tank reactor (CSTR) from Boudriga (1990) is used for this purpose. The system investigated in their study consists of a first-order sequential reaction, A → B → C, taking place in a nonisothermal CSTR. The process and the associated variables are illustrated in Figure 3, while the design equations are given below.

$$\tau = V/F \tag{4}$$

$$Q = F\rho C_P(T - T_i) + V(r_A H_{RA} + r_B H_{RB}) \tag{5}$$

$$C_A = \frac{C_{A_i}}{1 + k_A^0 e^{-E_A/(RT)}\tau} \tag{6}$$

$$C_B = \frac{C_{B_i} + k_A^0 e^{-E_A/(RT)}\tau C_A}{1 + K_B^0 e^{-E_B/(RT)}\tau} \tag{7}$$

$$-r_A = k_A^0 e^{-E_A/(RT)} C_A \tag{8}$$

$$-r_B = k_B^0 e^{-E_B/(RT)} C_B - k_A^0 e^{-E_A/(RT)} C_A \tag{9}$$

where V is the volume of the reactor, F is the volumetric flow rate, C_{A_i} and C_{B_i} are the inlet concentrations of A and B, C_A and C_B are the bulk concentrations of A and B. The rate of consumption of A and B are given by $-\tau_A$ and $-\tau_B$ and k_A^0, k_B^0 and E_A, E_B are the pre-exponential Arrhenius constants and activation energies respectively. Q is the rate of heat removal, T_i is the inlet temperatures of the reactants, T is the temperature of the material in the reactor, H_{RA} and H_{RB} are the molar heats of the reactions which are assumed to be independent of temperature and τ is the time constant of the CSTR. ρ and C_P represent the density and specific heats of the system which are assumed to be same for all processing streams.

The system parameters are given in Table 1. The design objective was to produce 60 mol/min of component B. The decision variables are chosen to be the inlet concentration of A (C_{Ai}), the inlet concentration of B (C_{Bi}), the inlet temperature (T_i), the reactor temperature (T), and the volume of the reactor (V). The error variables are assumed to be the inlet concentration of A (C_{Ai}), the inlet concentration of B (C_{Bi}), the inlet temperature (T_i), the reactor temperature (T), the volume of the reactor (V) and the flow rate (F).

Table 1. Parameters and Their Values Used in the Study

parameter	value	units
k_A^0	8.4×10^5	min^{-1}
k_B^0	7.6×10^4	min^{-1}
H_{RA}	-2.12×10^4	J/mol
H_{RB}	-6.36×10^4	J/mol
E_A	3.64×10^4	J/mol
E_B	3.46×10^4	J/mol
C_P	3.2×10^3	J/kg K
R	8.314	J/mol K
ρ	1180	kg/m^3

The nominal values of the parameters are calculated using the above objectives by solving the six equations (eqs 3–9). Boudriga (1990) studied parameter designs for this problem at various error levels using different approaches. We are using the same example to show the effect of different sampling techniques and number of samples on the accuracy of mean and variance predictions. Boudriga (1990) reported that in order to obtain reliable results for the mean and variance, a sample size of 1600 was necessary. As mentioned previously, the random Monte Carlo simulation technique was adopted in their analysis. In this study, we used the stochastic block to study the effects of different sampling techniques on the precision of the mean and variance of the output. The results are plotted in Figures 4 and 5 for the mean and variance, respectively. The figures also show the effect of differen random seeds. From the figures, it can be seen that the LHS technique always requires considerably less samples to converge to the right solution. It can also be seen that the mean is less affected by the number of samples or the sampling tecyhnique than the variance. For example, from Figures 4 and 5, it is apparent that to obtain consistent results within 2% of the exact value of the mean more than 3600 Monte Carlo samples are required unlike LHS which requires less than 100 samples. However, the same level of accuracy in variance predictions demands more than 1200 samples for LHS and much more than 5000 samples for MCS. Furthermore, the random seed changes the results of Monte Carlo simulations considerably for smaller sample size. This appears to be a big disadvantage of Monte Carlo simulations, especially for stochastic optimization problems. Normally, the random number generators started with a random seed automatically update the seed value for the next calculations. This means that the different iterations for optimization start at different random-seed values. If the random seeds change the results considerably as observed in Figures 4 and 5 for the Monte Carlo simulations, then the calculations of partial derivatives become erroneous, resulting in a failure of the optimization algorithm. To avoid this problem one has to resort to a large number of samples. Boudriga (1990) conducted several experiments for a specific set of nominal values of the parameters to arrive at the best value of the sample size. However, these experiments for one set of nominal values could be misleading as can be seen from the following example of calculating the precision of the mean.

An advantage of Monte Carlo techniques is that one can apply standard statistical techniques to calculate the precision of the estimate of the output distribution. For example, the estimate of mean value of the output value

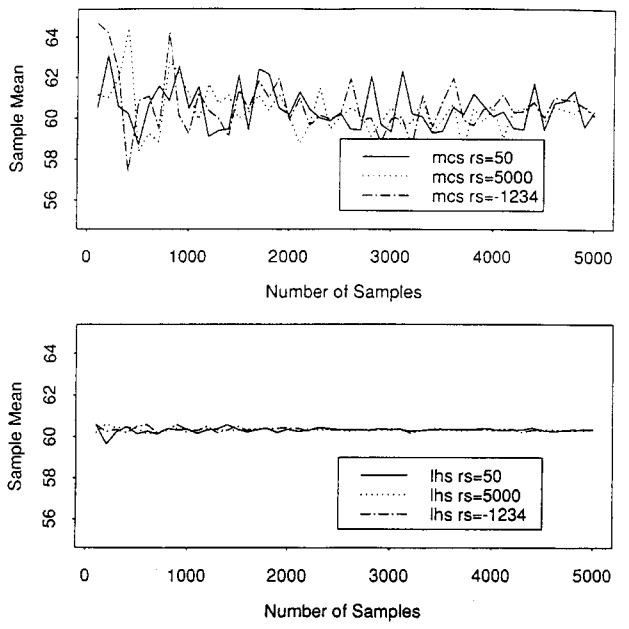


Figure 4. Comparison of MCS versus LHS, sample mean prediction.

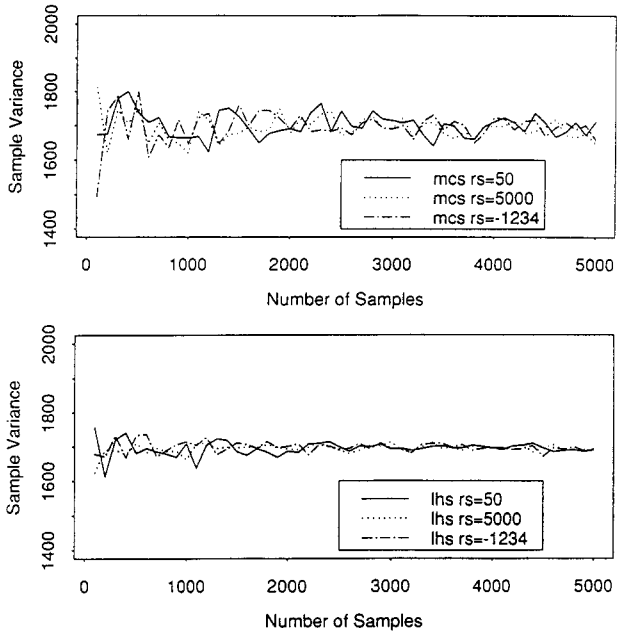


Figure 5. Comparison of MCS versus LHS, sample variance prediction.

y using m sample given by $\bar{y}$ is enclosed in an interval $(\bar{y} - c(\sigma/m^{1/2}), \bar{y} + c(\sigma/m^{1/2}))$ with the confidence α, where c is the standard deviation enclosing the probability α of the unit normal distribution. So, it can be seen that the number of samples required to obtain the given precision with high (e.g., $\alpha = 0.95$) confidence are dependent on the standard deviation σ. For further details on the precision calculations, the reader is referred to Morgan and Henrion (1990). Therefore, for different nominal values, the number of samples needed to predict the same accuracy can differ considerably, making it necessary to choose very large number of samples for a successful execution of the optimization algorithm. The LHS, on the other hand, provides a means for circumventing this problem.

6. Parameter Design of a Simple Flowsheet

As an illustration of the parameter design methodology, a simple flowsheet (Figure 6a) consisting of a compressor

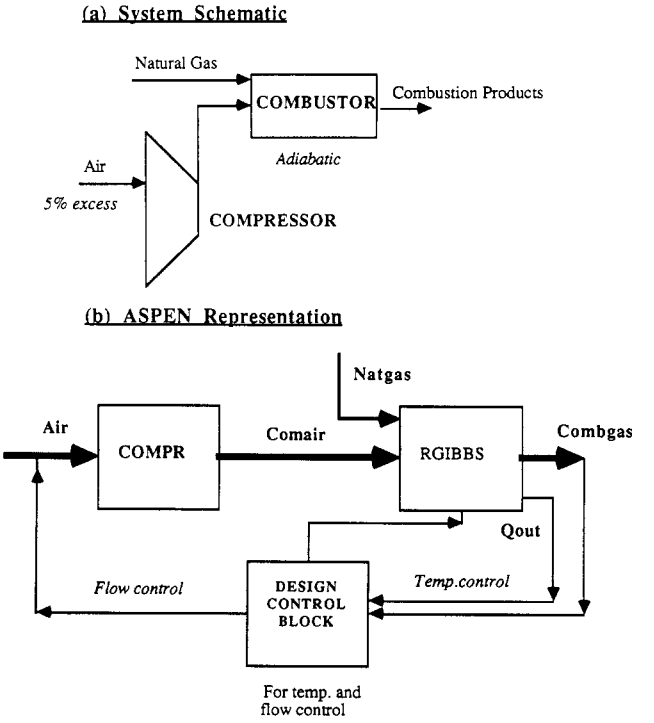


Figure 6. Process flowsheet of a simple system.

and a natural gas combustor is considered. In this flowsheet, air is first passed through the compressor, and then through the combustor where fuel is added and the combustion reaction takes place. The reactor is assumed to be adiabatic. Figure 6b shows the ASPEN representation of the flowsheet along with the parameter design framework. The flowsheet uses the compressor block for air compression. For the combustor, the ASPEN reactor model based on the concept of minimum Gibbs free energy, is employed. To simulate adiabatic operation of the reactor, a design specification block is used. This block adjusts the reactor temperature to achieve zero net heat transfer. The air flow is always maintained to supply 5% excess oxygen by using an additional design specificatino block.

Three input parameters—the fuel flow rate (F_{NG}), the compressor pressure (P_{CMP}) and the combustor pressure drop (ΔP)—are assumed to be the error variables as well as the decision variables whose nominal values are to be adjusted using the parameter design methodology. The decision variables are subject to the following inequality constraints.

$$4.0 \text{ lb mol/h} \le F_{NG} \le 10.0 \text{ lb mol/h} \quad (10)$$

$$100.0 \text{ psia} \le P_{CMP} \le 160.0 \text{ psia} \quad (11)$$

$$-10.0 \text{ psia} \le \Delta P \le -4.0 \text{ psia} \quad (12)$$

The air flow rate is chosen as the output parameter whose variability needs to be controlled using this off-line quality control method. Figure 7 shows the initial probability distributions (solid lines) with 8% error in the variables. It was found that 50 samples were sufficient to obtain stable stochastic optimization results for this example. Figure 7 shows the resulting distribution (dotted lines) after the optimal nominal values are selected by the parameter design framework. It may be noted that with the proposed framework it was possible to reduce the variance of the flow rate from 963 to 142, by merely

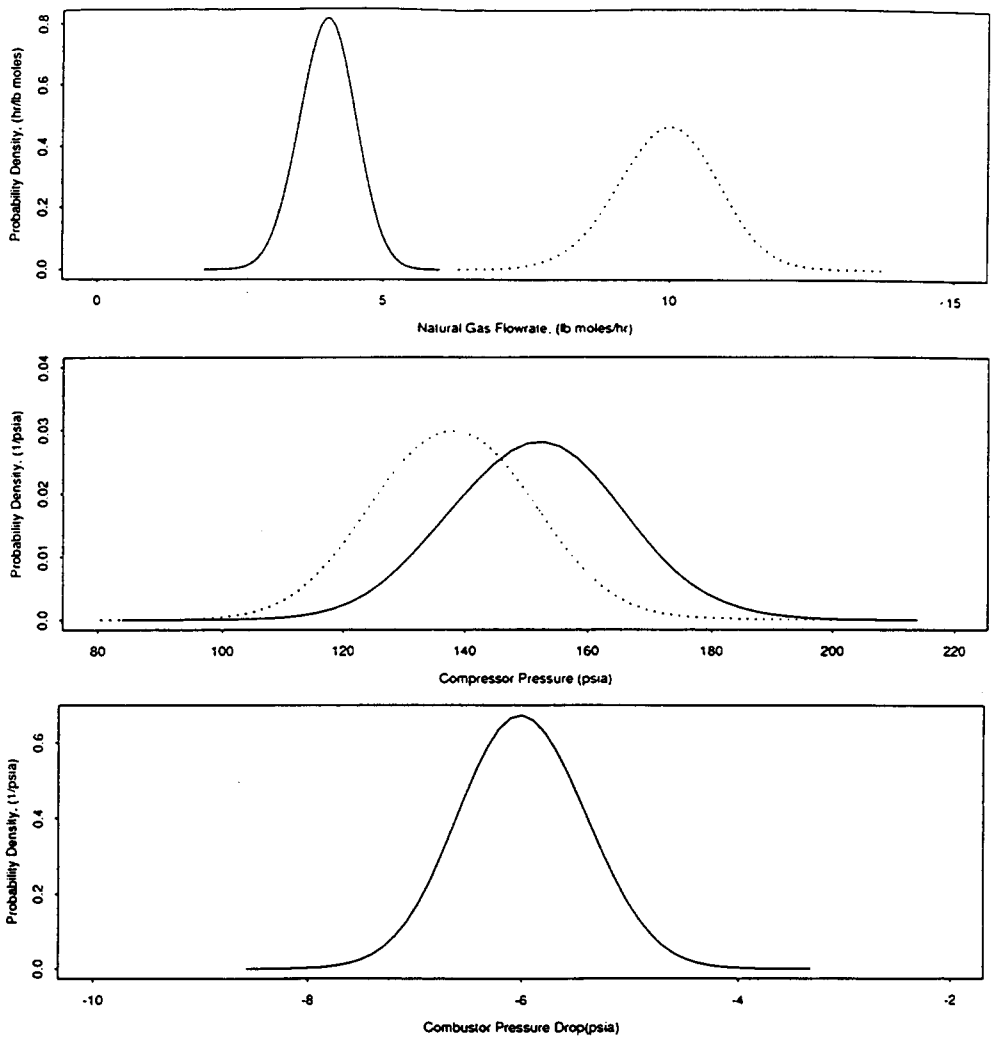


Figure 7. Input distributions before parameter design (solid line) and after parameter design (dotted line).

changing the nominal values of the two sensitive parameters, F_{NG} and P_{CMP}.

The major bottleneck in stochastic optimization, especially for large-scale industrial problems (with the current capability, it is possible to solve any large-scale problem with maximum of 100 error variables), is the enormous computational time required. For example, a typical chemical process may have 15–20 noisy or uncertain variables demanding at least 1000–2000 LHS samples per optimization run. Although the present approach using efficient sampling techniques reduces the computational time relative to the other approaches, it still leaves much to be attained in terms of an absolute computational efficiency. A new algorithm based on the derivative information obtained from response surface methodology shows promise for reducing the CPU time considerably and can provide better partial derivatives to the optimizer than the perturbation method. This method will be explored in a future work.

7. Conclusions

This paper presented a generalized framework for implementation of the parameter design method for chemical processes. The framework centered around the ASPEN chemical process simulator and employed stochastic optimization techniques. The paper also explored the effect of different sampling techniques on the precision of the results. It was found that Latin hypercube sampling is always preferred in parameter design method because of its high precision and consistent behavior. The parameter design method was illustrated using a small chemical plant flowsheet. A future work will address the problem of increasing computational efficiency of the stochastic optimization by using the response surface method for calculation of derivatives.

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Nomenclature

C_A = the bulk concentrations of A, mol/m^3
C_{Ai} = the initial concentrations of A, mol/m^3
C_B = the bulk concentrations of B, mol/m^3
C_{Bi} = the initial concentrations of B, mol/m^3
C_P = specific heat of the system, J/kg K
E = the error level, %
E_A = the activation energy of the first reaction, J/mol
E_B = the activation energy of the second reaction, J/mol
F = the volumetric flow rate, m^3/min
F_{NG} = the fuel flow rate, lb moles/h
H_{RA} = molar heat of the first reaction, J/mol
H_{RB} = molar heat of the second reaction, J/mol

k_A^0 = the preexponential Arrhenius constants for the first reaction, min^{-1}
k_B^0 = the pre-exponential Arrhenius constants for the second reaction, min^{-1}
nv = number of decision variables
N = number of samples
P_{CMP} = the compressor pressure, psia
ΔP = the combustor pressure drop, psia
Q = the rate of heat removal, J/min
$-\tau_A$ = the rate of disappearance of A, mol/(m^3 min)
$-\tau_B$ = the rate of disappearance of B, mol/(m^3 min)
T = the temperature of the material in the reactor, K
T_i = the inlet temperatures of the reactors, K
V = the volume of the reactor, m^3
y_i = the output variable corresponding to sample i
$\bar{y}$ = the average of the output values

Greek Symbols

μ_i = nominal value of the input variable i
ρ = density of the system, kg/m^3
σ_i = standard deviation of the input variable i
σ_o = standard deviation of the output
σ_o^2 = variance of the output
τ = the time constant of the CSTR, min

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