Chinese J. Chem. Eng., 12 (5) 673 – 676 (2004)

A Modified Model for Flexibility Analysis in Chemical Engineering Processes

ZHANG Lei(张蕾), HE Xiaorong(何小荣)* and XU Qiang(徐强)
Department of Chemical Engineering, Tsinghua University, Beijing 100084, China

Abstract This paper discussed an extended model for flexibility analysis of chemical process. Under uncertainty, probability density function is used to describe uncertain parameters instead of hyper-rectangle, and chance-constrained programming is a feasible way to deal with the violation of constraints. Because the feasible region of control variables would change along with uncertain parameters, its smallest acceptable size threshold is presented to ensure the controllability condition. By synthesizing the considerations mentioned above, a modified model can describe the flexibility analysis problem more exactly. Then a hybrid algorithm, which integrates stochastic simulation and genetic algorithm, is applied to solve this model and maximize the flexibility region. Both numerical and chemical process examples are presented to demonstrate the effectiveness of the method.
Keywords flexibility analysis, chance-constrained programming, stochastic simulation, genetic algorithm

1 INTRODUCTION

Flexibility of a chemical process is the ability of the system to maintain feasible steady-state operation over a range of uncertain operating environments. It is one of the key components of chemical plant operability[1,2]. Flexibility analysis in process synthesis under uncertainty has become an important part of process system engineering research. The practical operating conditions must be avoided to be far from the fixed design ones such that the operation will violate the process constraints caused by the fluctuation of the uncertain factor. A lot of systematic work in this field has been presented, which involved process modeling, optimization procedure and solution strategy. Some studies discussed theoretical developments[3] and effective calculation method[4,5], some focused on the combination of flexibility and reliability, controllability, robustness and safety for chemical processes[6,7]. This paper attempts to discuss several sub-problems about uncertainty and controllability in flexibility analysis, and to propose more appropriate way of modeling practical processes. Then, an integrated algorithm is suggested to solve the optimization problem about determining the flexibility region.

2 UNCERTAIN PARAMETERS

Flexibility analysis gives consideration to the uncertain parameters in the design and actual operation of chemical plants which include either internal process parameters such as stream flow rate, stream specifications, operation temperature and transfer coefficients, or external process parameters such as feed quality, economic cost data, and product price[8]. These uncertain parameters are denoted by vector $\boldsymbol{\theta}$. Similarly, $\boldsymbol{d}$ is the vector of design variables which remain fixed during the process operation, vector $\boldsymbol{x}$ represents the state variables, and control variables vector $\boldsymbol{z}$ represents the degree of operation freedom that can eliminate the system fluctuation occurred by the uncertain parameters. A steady state of chemical process can be described by using these symbols

$$\begin{aligned} \boldsymbol{h}(\boldsymbol{d},\boldsymbol{z},\boldsymbol{x},\boldsymbol{\theta}) &= 0 \\ \boldsymbol{g}(\boldsymbol{d},\boldsymbol{z},\boldsymbol{x},\boldsymbol{\theta}) &\leqslant 0 \end{aligned} \tag{1}$$

By eliminating the state variables $\boldsymbol{x}$, the process state can be described by the following reduced inequality constraints

$$\begin{aligned} \boldsymbol{h}(\boldsymbol{d},\boldsymbol{z},\boldsymbol{x},\boldsymbol{\theta}) = 0 &\Longrightarrow \boldsymbol{x} = \boldsymbol{x}(\boldsymbol{d},\boldsymbol{z},\boldsymbol{\theta}) \\ \boldsymbol{g}[\boldsymbol{d},\boldsymbol{z},\boldsymbol{x}(\boldsymbol{d},\boldsymbol{z},\boldsymbol{\theta}),\boldsymbol{\theta}] &= \boldsymbol{f}(\boldsymbol{d},\boldsymbol{z},\boldsymbol{\theta}) \leqslant 0 \end{aligned} \tag{2}$$

Hyper-rectangle is a classic means to describe the range of $\boldsymbol{\theta}$. Giving the nominal point $\boldsymbol{\theta}^{\mathrm{N}}$, two corresponding sides displaced proportional to the expected positive and negative deviations $\Delta\boldsymbol{\theta}^{+}$, $\Delta\boldsymbol{\theta}^{-}$ and the scalar parameter δ (mainly based on experience), the range of $\boldsymbol{\theta}$ is

$$T(\delta) = \{\boldsymbol{\theta} | \boldsymbol{\theta}^{\mathrm{N}} - \delta\Delta\boldsymbol{\theta}^{-} \leqslant \boldsymbol{\theta} \leqslant \boldsymbol{\theta}^{\mathrm{N}} + \delta\Delta\boldsymbol{\theta}^{+}\} \tag{3}$$

This hyper-rectangle determines the actual size of the region for feasible operation in the space of uncertain parameters. It is one of the bases of "flexibility index"[1,2] and "active constraint strategy" methods[9]. Xu extended the hyper-rectangle description method into "local adjusting method" for flexibility region of chemical process[10], where the range of $\boldsymbol{\theta}$ is

$$T(\delta) = \{\boldsymbol{\theta} | \theta_i^{\mathrm{N}} - \delta_i^{-}\Delta\theta_i^{-} \leqslant \theta_i \leqslant \theta_i^{\mathrm{N}} + \delta_i^{+}\Delta\theta_i^{+},\ i = 1,\cdots,I\} \tag{4}$$

These above methods, however, are all based on an assumption that all the uncertain parameters have uniform distribution, which does not accord with the practice that different parameter is subject to different

Received 2003-07-21, accepted 2004-06-21.
* To whom correspondence should be addressed. E-mail: hexr@mail.tsinghua.edu.cn

distribution. So it is better to use probability density function to describe each uncertain parameter

$$T(\boldsymbol{\theta}) = \{\boldsymbol{\theta}|\theta_i \sim pdf_i(a_{i1}, a_{i2}, \cdots), \quad i = 1, \cdots, I\} \quad (5)$$

where pdf_i is the probability density function of variable θ_i, a_{nm} is the function parameter. In practical problems, the familiar distributions of chemical process parameters may include uniform, normal, triangular, exponential, and so on. They should be decided individually by domain knowledge and experience.

3 CONSTRAINTS UNDER THE UNCERTAIN ENVIRONMENT

In a system with uncertain parameters, it is of course ideal for the operation to satisfy all the constraints. The investment and operation cost of process may be very expensive in order to avoid any violation of constraints completely. In fact, the constraints in process industry can be classified into two classes depending on whether the violations caused by the uncertainty are acceptable. Constraints that must not be violated under any circumstance are classified as "hard" ones, the equipment safety limitation for example. On the other hand, some constraints are "soft" and their violation can be tolerated, *e.g.* the product specifications[11].

The chance-constrained programming could be useful to deal with different types of constraints. When uncertain parameters exist in constraints, chance-constrained programming can provide a powerful means of modeling a stochastic decision system with assumption that stochastic constraint will hold at least α of time, where α is the confidence level provided as an appropriate parameters by user. Then the inequality constraints (2) become

$$Pr\{f_i(\boldsymbol{d}, \boldsymbol{z}, \boldsymbol{\theta}) \leqslant 0, \quad i \in I\} \geqslant \alpha \quad (6)$$

where $Pr\{*\}$ denotes the probability of the events in { }. Solving chance-constrained programming directly by stochastic simulation and some heuristic optimization algorithm such as genetic algorithm has become feasible and effective now, along with rapid development of computer tools[12].

4 FEASIBLE REGION LIMITATION OF CONTROL VARIABLES

Let's consider an example from the practical chemical process, which is given by Swaney[1,2] and used also by other authors[10]. It describes the liquid transportation by a centrifugal pump, whose data are shown in Table 1, and state constraint is inequality Eq. (7).

$$\begin{aligned}
&\left(p_1 + \rho H - \frac{m^2}{\rho C_{\mathrm{V}}^2} - k m^{1.84} D^{-5.16}\right) - p_2^* - \varepsilon \leqslant 0 \\
&-\left(p_1 + \rho H - \frac{m^2}{\rho C_{\mathrm{V}}^2} - k m^{1.84} D^{-5.16}\right) + p_2^* - \varepsilon \leqslant 0 \\
&mH - \eta W \leqslant 0 \\
&C_{\mathrm{V}} - C_{\mathrm{V}}^{\mathrm{MAX}} \leqslant 0 \\
&r C_{\mathrm{V}}^{\mathrm{MAX}} - C_{\mathrm{V}} \leqslant 0
\end{aligned} \quad (7)$$

The feasible hyper-rectangle result obtained by the extended local adjusting method[10] is

$$\begin{aligned} 232.461 \leqslant p_2^* \leqslant 906.650 \\ 4.841 \leqslant m \leqslant 11.067 \end{aligned} \quad (8)$$

According to constraint Eq. (7) and flexibility region Eq. (8), we can get Fig. 1. It is a 3-D graph that describes the relation between feasible region of control variable and uncertain parameters. The x-axes and y-axes denote two uncertain parameters p_2^* and m, respectively. The z-axes denote the sizes of feasible region of control variable C_{V}, which ensure the constraints can be hold. Fig. 2 is a contour plot enlarging a part of surface in Fig. 1.

In order to satisfy the constraints as high as possible, control variables must be adjusted with different realization of uncertain parameters. Apparently, the adjustable range, or the feasible region size of control variable, is also different with different realization of uncertain parameters. Sometimes the control variable

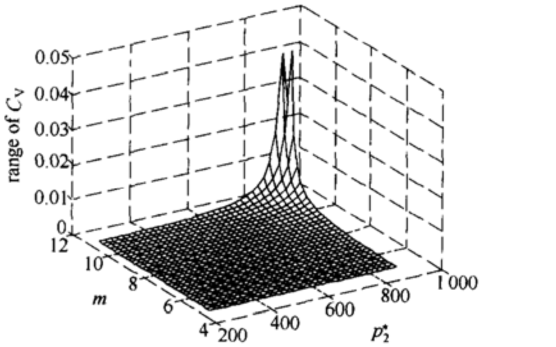

Figure 1 Relationship between control variable and uncertain parameters

Table 1 Data of pump system in example

Design variable	Process constant	Values of uncertain parameter
driving power: $W = 35\,\mathrm{kW}$	pump efficiency: $\eta = 0.5$	
pump head: $H = 1.4\,\mathrm{kJ \cdot kg^{-1}}$	lower limit coefficient of control	desired pressure: $p_2^{*\mathrm{N}} = 800\,\mathrm{kPa}$
pipe diameter:	valve: $r = 0.05$	$\Delta p_2^{*+} = 200\,\mathrm{kPa}$
$D = 0.072\,\mathrm{m}$	liquid density: $\rho = 1000\,\mathrm{kg \cdot m^{-3}}$	$\Delta p_2^{*-} = 550\,\mathrm{kPa}$
upper bound of control	source pressure: $p_1 = 100\,\mathrm{kPa}$	liquid flowrate: $m^{\mathrm{N}} = 10\,\mathrm{m \cdot s^{-1}}$
valve size:	pressure drop constant: $k = 9.101 \times 10^{-6}\,\mathrm{kPa}$	$\Delta m^+ = 2\,\mathrm{m \cdot s^{-1}}$
$C_{\mathrm{V}}^{\mathrm{MAX}} = 0.09$	tolerance of p_2^*: $\varepsilon = 20\,\mathrm{kPa}$	$\Delta m^- = 5\,\mathrm{m \cdot s^{-1}}$

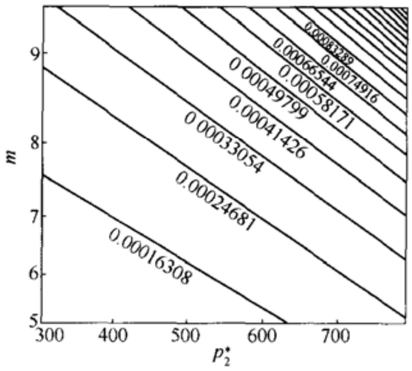

Figure 2 Contour plot of feasible region of C_V

may be limited in a very strict range, for example, in the most area in Fig. 1. It is more clearly in Fig. 2. The statistical result of the feasible region size of control variable is shown in Table 2. Though they are theoretical feasible solutions, it will be very difficult or even impossible to set the control variable within an extreme small region in real producing process.

Table 2 Distribution of feasible region of C_V

Feasible region size of C_V (RC_V)	Area percentage, %
$RC_V \leqslant 0.0001$	1.63
$0.0001 < RC_V \leqslant 0.0002$	21.60
$0.0002 < RC_V \leqslant 0.0004$	34.21
$0.0004 < RC_V \leqslant 0.0007$	20.44
$0.0007 < RC_V \leqslant 0.005$	20.15
$RC_V > 0.005$	1.97

To solve this problem which is adverse to controllability, we enhance the constraint

$$Pr\{f_i(\boldsymbol{d}, \hat{\boldsymbol{z}}, \boldsymbol{\theta}) \leqslant 0, i \in I\} \geqslant \alpha, \forall \hat{\boldsymbol{z}} \in [\boldsymbol{z} - \Delta \boldsymbol{z}, \boldsymbol{z} + \Delta \boldsymbol{z}] \tag{9}$$

where $\Delta \boldsymbol{z}$ is the deviation which describes the smallest acceptable bound of feasible region size of $\boldsymbol{z}$, given by user. Thus, the enhanced constraint can ensure a feasible region size of $\boldsymbol{z}$ that is greater than setting threshold, with any possible $\boldsymbol{\theta}$. This region of $\boldsymbol{z}$ should be attainable in actual operation.

5 INTEGRATED ALGORITHM OF FLEXIBILITY ANALYSIS

By synthesizing the three sections above and setting an objective function correlate with flexibility, the flexibility analysis in chemical engineering processes will become a chance-constrained programming. Then we integrate a hybrid intelligent algorithm to solve this optimization problem and to get the flexibility feasible region. The brief procedure is listed as follows

Step 1. Model the flexibility analysis problem by using chance-constrained programming and other methods, and initialize the parameters.

Step 2. Generate feasible solution for uncertain constraints by stochastic simulation.

Step 3. Get the optimal solution through selection, crossover and mutation of genetic algorithm, and then report it.

6 EXAMPLES

Firstly, consider a numerical example which involves five constraints with one control variable z and two uncertain parameters θ_1 and θ_2. Design variables are omitted. The optimization form of this problem is:

$$\begin{aligned}
&\max A \\
&s.t. \\
&Pr\{f_1 = z - \theta_1 + 2\theta_2 - 11 \leqslant 0\} \geqslant 0.97 \\
&Pr\{f_2 = -z - 0.5\theta_1 - \theta_2 + 6 \leqslant 0\} \geqslant 0.95 \\
&Pr\{f_3 = z + \theta_1 - \theta_2 - 12 \leqslant 0\} \geqslant 0.98 \\
&Pr\{f_4 = z + 2\theta_1 + 3\theta_2 - 25 \leqslant 0\} \geqslant 0.99 \\
&Pr\{f_5 = -z + 0.2\theta_1 - 2\theta_2 + 11 \leqslant 0\} \geqslant 0.96 \\
&-20 \leqslant z \leqslant 30 \\
&\theta_1 \sim N(2, 5^2), \theta_2 \sim T(-6, 13, 4)
\end{aligned} \tag{10}$$

where A is the area of feasible rectangle in the space of uncertain parameters, $N(\mu, \sigma^2)$ is normal probability density function, $T(a, b, m)$ is triangular probability density function.

The final result of the problem by using integrated algorithm is shown in Fig. 3 and inequality Eq. (11). The hyper-rectangle of flexibility region is larger than the feasible region indicated by dashed line, because the constraints can be violent in the given probability.

$$\begin{aligned}
-0.498 \leqslant \theta_1 \leqslant 3.781 \\
-0.107 \leqslant \theta_2 \leqslant 6.253
\end{aligned} \tag{11}$$

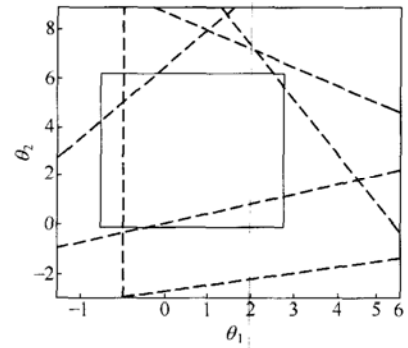

Figure 3 Flexibility region of numerical example

The second example is still one about the pump system with some additional setting

$$\begin{aligned}
&\max A \\
&s.t. \\
&\left(p_1 + \rho H - \frac{m^2}{\rho \hat{C}_V^2} - km^{1.84} D^{5.16}\right) - p_2^* - \varepsilon \leqslant 0 \\
&-\left(p_1 + \rho H - \frac{m^2}{\rho \hat{C}_V^2} - km^{1.84} D^{5.16}\right) + p_2^* - \varepsilon \leqslant 0 \\
&mH - \eta W \leqslant 0 \\
&\hat{C}_V - C_V^{MAX} \leqslant 0 \\
&rC_V^{MAX} - \hat{C}_V \leqslant 0 \\
&p_2^* \geqslant 200 \\
&\forall \hat{C}_V \in [C_V - \Delta C_V, C_V + \Delta C_V], \Delta C_V = 0.00005 \\
&p_2^* \sim U(0, 1500), m \sim U(0, 15)
\end{aligned} \tag{12}$$

Considering the feature of problem and the convenience of result comparison, uniform probability density function, $U(a,b)$, is selected to describe both stochastic parameters. The object is to maximize the area of the feasible region. By the integrated algorithm, we get the result of feasible region as follows

$$\begin{aligned} 200.000 \leqslant p_2^* \leqslant 833.771 \\ 5.875 \leqslant m \leqslant 11.770 \end{aligned} \tag{13}$$

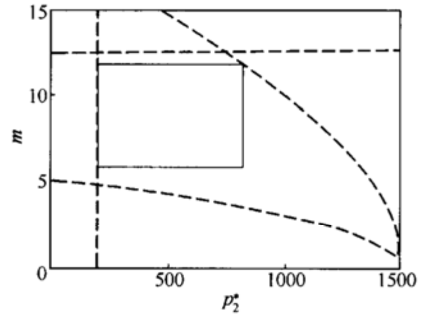

Figure 4 Flexibility region of the pump system

The flexibility hyper-rectangle is not fully filled in the feasible region. In some area nearby the feasible bounds, the range of control variable corresponding to the uncertainty may be too strict to be realized in real operation. This area is eliminated from the result.

In these examples, the chance-constrained programming extends the flexibility region, while the feasible regions limitations of control variables reduce it. Though they have inverse apparent effect, they all describe some aspects of the practical problems.

7 CONCLUSIONS

The paper compares probability density function method with hyper-rectangle in uncertain parameters description, confirms that the former is more effective to actual process. By considering the safety of constraints, the flexibility model modified by chance-constraint programming can work on different conditions. The problem about controllability is solved by introducing new enhanced constraint. To solve this optimization problem of flexibility analysis based on modified model, an integrated algorithm including stochastic simulation and genetic algorithm is suggested. Because the advantage of heuristics, this optimization algorithm can deal with various complicated cases. The sample calculation and analysis indicate the modified model and corresponding solving algorithm is more practical and trustworthy to chemical process design and operation.

NOMENCLATURE

a_{nm}	parameter of probability density function
$\boldsymbol{d}$	vector of design variables
f	reduced inequality constraints
g	original inequality constraints
h	original equality constraints
$Pr\{\ \}$	probability of the events in $\{\ \}$
pdf	probability density function
$T(\delta)$	hyperrectangle with scalar variable δ
$T(\boldsymbol{\theta})$	hyperrectangle with distribution of $\boldsymbol{\theta}$
$\boldsymbol{x}$	vector of state variables
$\boldsymbol{z}$	vector of control variables
$\hat{\boldsymbol{z}}$	active value of z
$\Delta\boldsymbol{z}$	deviation of control variables
α	confidence level
δ	scaled parameter deviation
δ^+	scaled parameter positive deviation
δ^-	scaled parameter negative deviation
$\boldsymbol{\theta}$	vector of uncertain parameters
$\boldsymbol{\theta}^{\mathrm{N}}$	nominal point of vector $\boldsymbol{\theta}$
$\Delta\boldsymbol{\theta}^+$	positive deviation of vector $\boldsymbol{\theta}$
$\Delta\boldsymbol{\theta}^-$	negative deviation of vector $\boldsymbol{\theta}$

REFERENCES

1 Swaney, R.E., Grossmann, I.E., "An index for operational flexibility in chemical process design, Part I: Formulation and theory", *AIChE J.*, **31** (4), 621—630 (1985).

2 Swaney, R.E., Grossmann, I.E., "An index for operational flexibility in chemical process design, Part II: Computational algorithms", *AIChE J.*, **31** (4), 631—641 (1985).

3 Bansal, V., Perkins, J.D., Pistikopoulos, E.N., "Flexibility analysis and design of dynamic processes with stochastic parameters", *Comput. Chem. Eng.*, **22** (suppl.), 817—820 (1998).

4 Ostrovsky, G.M., Volin, Y.M., Golovashkin, D.V., "Optimization problem of complex system under uncertainty", *Comput. Chem. Eng.*, **22** (7—8), 1007—1015 (1998).

5 Raspanti, C.G., Bandoni, J.A., Biegler, L.T., "New strategies for flexibility analysis and design under uncertainty", *Comput. Chem. Eng.*, **24**, 2193—2209 (2000).

6 Michael, C.G., Efstratios, N.P., "An integrated framework for robust and flexible process systems, robust process planning under uncertainty", *Ind. Eng. Chem. Res.*, **38** (1), 133—143 (1999).

7 Shabbir, A., Nikolaos, V.S., "Robust process planning under uncertainty", *Ind. Eng. Chem. Res.*, **37** (5), 1883—1892 (1998).

8 Halemane, K.P., Grossmann, I.E., "Optimal process design under uncertainty", *AIChE J.*, **29** (3), 425—433 (1983).

9 Grossmann, I.E., Floudas, C.A., "Active Constraint strategy for flexibility analysis in chemical process", *Comput. Chem. Eng.*, **11** (6), 675—683 (1987).

10 Xu, Q., Chen, B.Z., He, X.R., "An extended algorithm of flexibility analysis in chemical engineering process", *Chinese J. Chem. Eng.*, **9** (1), 51—57 (2001).

11 Samsatli, N.J., Papageorgiou, L.G., Shah, N., "Robustness metrics for dynamic optimization models under parameter uncertainty", *AIChE J.*, **44** (4), 1993—2005 (1993).

12 Liu, B.D., Zhao, R.Q., Stochastic Programming and Fuzzy Programming, Tsinghua University Press, Beijing (1998). (in Chinese)