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# An Extended Algorithm of Flexibility Analysis in Chemical Engineering Processes

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**Abstract** An extended algorithm of flexibility analysis with a local adjusting method for flexibility region of chemical processes, which is based on the active constraint strategy, is proposed, which fully exploits the flexibility region of the process system operation. The hyperrectangular flexibility region determined by the extended algorithm is larger than that calculated by the previous algorithms. The limitation of the proposed algorithm due to imperfect convexity and its corresponding verification measure are also discussed. Both numerical and actual chemical process examples are presented to demonstrate the effectiveness of the new algorithm.
**Keywords** flexibility analysis, extended algorithm, active constraint strategy

## 1 INTRODUCTION

Flexibility of a chemical plant design is the ability of the designed chemical process to maintain feasible steady-state operation over a range of uncertain operating conditions. In the design and actual operation of chemical plants, much consideration should be given to the uncertain parameters, which vary frequently during the process operation. The sources of uncertainties may be either internal process parameters such as stream flowrate, stream specifications, operation temperature and transfer coefficients, or external process parameters such as the feed quality, economic cost data, and product price[1]. As we all know, the optimal process design based on one set of fixed operating conditions does not always perform well in actual operation, because the fluctuation of the uncertain parameters may cause the practical operating conditions far from the design ones such that the operation violates the process constraints. That is why flexibility analysis in process synthesis under uncertainty has become a most active topic in process system engineering research in the last two decades. With the social and technological development the number of uncertainties which may influence the profitability of chemical plants will increase gradually. This makes the flexibility analysis remaining a key factor in future process synthesis.

Flexibility analysis in chemical process is a rather difficult task, which involves process modeling, optimization procedure and solving strategy for a large scale system with nonlinear constraints. We have reported the results on structural flexibility for heat integrated distillation columns[2] and flexibility analysis for heat exchange network[3]. Other authors also presented their excellent systematic work[4–11] in this field. At present the flexibility analysis is focused on the combination of flexibility and reliability, controllability, robustness and safety for chemical processes[4–6], which would result in improved operability of chemical plants in an extended view of process system engineering.

For a chemical process system designed with a set of fixed parameters, an important theoretic and actual consideration is how to determine the flexibility region in the space of uncertain parameters for this chemical process system. Swaney[7,8] proposed the concept of "flexibility index", which provided a general framework for measuring the size of the region of feasible operation. The solution methods with consideration of particular conditions were also given. Then Grossmann[9], based on the "flexibility index", proposed "the active constraint strategy" which provided a general mixed-integer optimization method to determine the actual size of the region for feasible operation in the space of uncertainty parameters. These methods give a quantitative measure for the hyperrectangle used to characterize the flexibility region of the uncertainties, which is very useful for practical chemical process. The above methods, however, are all based on a special assumption that the positive and negative deviations of all the uncertain parameters have the equal scalar value for their own expected deviations. It then results in that the hyperrectangle calculated by the previous methods was considerably conservative and could not exploit in most cases the maximum flexibility region over which the process could maintain the feasible operation. It is the objective of this paper to present a new extended algorithm to generate the maximum flexibility hyperrectangle for a chemical process system. The algorithm incorporates with the

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method of locally adjusted hyperrectangle, which was based on the active constraint strategy for flexibility analysis[9]. The paper also discussed the limitation of the algorithm and its corresponding checking measure. Before introducing the new algorithm, the basic concepts of "flexibility index" and method of active constraint strategy would be briefly interpreted.

## 2 FLEXIBILITY INDEX AND ACTIVE CONSTRAINT STRATEGY

The variables of a chemical process with uncertainty can be classified into four categories. The vector design variables of $\boldsymbol{d}$ is associated with equipment size, which remain fixed during the operation of the plant once the design is completed. The vector $\boldsymbol{x}$ corresponds to the state variables which are determined by solving the set of equations representing the process system. $\boldsymbol{\theta}$ is the vector of uncertain parameters of the process system. The vector $\boldsymbol{z}$ of control variables represents the degrees of operation freedom that can be adjusted for different realization of $\boldsymbol{\theta}$. Using these variables a steady state of chemical process is described by the following sets of equalities and inequalities constraints

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

For a given design $\boldsymbol{d}$ and for any realization of $\boldsymbol{\theta}$, the state variables is generally expressed as an implicit function of the control $\boldsymbol{z}$ using the equalities $\boldsymbol{h}$. This allows the elimination of state variables so that the process is described by the following reduced inequality constraints

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

The range of $\boldsymbol{\theta}$ (flexibility region) may be described as a hyperrectangle $T$ which is centered at the nominal point $\boldsymbol{\theta}^{\mathrm{N}}$ with two corresponding sides displaced proportional to the expected positive and negative deviations $\Delta\boldsymbol{\theta}^{+}$, $\Delta\boldsymbol{\theta}^{-}$ (estimated based on experience or rule-of-thumb target values[7]).

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

where the scalar parameter $\boldsymbol{\delta}$ determines the practical range of $\boldsymbol{\theta}$ over which the chemical process operation is feasible. It should be noted that the control vector of $\boldsymbol{z}$ is adjusted during the operation to guarantee that the process constraints in Eq. (2) are satisfied for any realization of $\boldsymbol{\theta}$ in $\boldsymbol{T}(\delta)$. For a fixed $\delta$, the process constraints may be reformulated as the following form[1]

$$\max_{\boldsymbol{\theta}\in\boldsymbol{T}(\delta)}\min_{\boldsymbol{z}}\max_{i\in I}f_i(\boldsymbol{d},\boldsymbol{z},\boldsymbol{\theta})\leqslant 0 \tag{4}$$

where $I$ is the index set for the inequalities. The direct solution of problem with Eq. (4) is very difficult due to the max-min-max constraint. In order to get the insight of constraint (4), $\boldsymbol{\Psi}(\boldsymbol{d},\boldsymbol{\theta})$ is introduced to decompose the max-min-max constraint into

$$\max_{\boldsymbol{\theta}\in\boldsymbol{T}(\delta)}\boldsymbol{\Psi}(\boldsymbol{d},\boldsymbol{\theta})\leqslant 0 \tag{5}$$

$$\begin{aligned} &\boldsymbol{\Psi}(\boldsymbol{d},\boldsymbol{\theta})=\min_{u,\boldsymbol{z}}u \\ \text{s.t.}\quad &f_i(\boldsymbol{d},\boldsymbol{z},\boldsymbol{\theta})\leqslant u,\quad i\in I \end{aligned} \tag{6}$$

The solution of above problem is the projection of process feasible region in space $\boldsymbol{\theta}$. For fixed $\boldsymbol{d}$, two dimensions of $\boldsymbol{\theta}$, the process feasible region made up by $\boldsymbol{\Psi}(\boldsymbol{d},\boldsymbol{\theta})\leqslant 0$ and flexibility region represented by a hyperrectangle $\boldsymbol{T}(\delta)$ are shown in Fig. 1. It should be noted that for convex feasible region, the critical point which limits the outspread size of $\boldsymbol{T}(\delta)$ always lies at one of its vertices. While for nonconvex region, it needs a specific analysis from case to case. In practical chemical processes, however, an empirical intuition suggests that the critical point lies at a vertex[7].

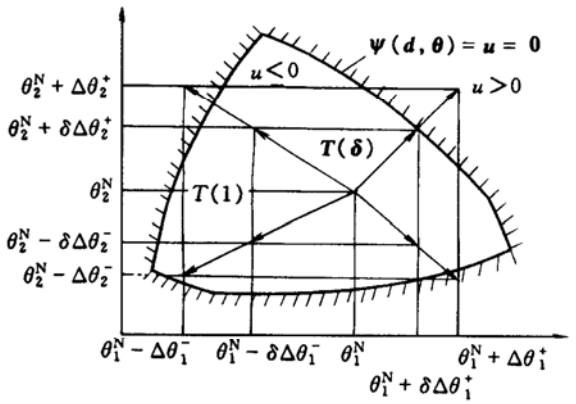


**Figure 1 Feasible region and flexibility $\boldsymbol{T}(\delta)$**

For a given design $\boldsymbol{d}$, the flexibility index $\boldsymbol{F}$ is defined by the maximum obtained from the programming problem Eq. (7)[7]. As shown in Fig. 1, $\delta$ represents the measure of the largest hyperrectangle inscribed in the feasible region.

$$\begin{aligned} &F=\max\delta \\ \text{s.t.}\quad &\max_{\boldsymbol{\theta}\in\boldsymbol{T}(\delta)}\min_{\boldsymbol{z}}\max_{i\in I}f_i(\boldsymbol{d},\boldsymbol{z},\boldsymbol{\theta})\leqslant 0 \\ &\boldsymbol{T}(\delta)=\left\{\boldsymbol{\theta}\middle|\boldsymbol{\theta}^{\mathrm{N}}-\delta\Delta\boldsymbol{\theta}^{-}\leqslant\boldsymbol{\theta}\leqslant\boldsymbol{\theta}^{\mathrm{N}}+\delta\Delta\boldsymbol{\theta}^{+}\right\} \end{aligned} \tag{7}$$

Using the active constraint strategy to solve above problem leads to the following mixed-integer optimization programming[9]

$$F = \min\delta$$

s.t.

$$\begin{cases} f_i(\boldsymbol{d}, \boldsymbol{z}, \boldsymbol{\theta}) + s_i = 0 \\ \sum_i \lambda_i + 1 \\ \sum_i \lambda_i \dfrac{\partial f_i}{\partial \boldsymbol{z}} = 0 \\ \lambda_i - y_i \leqslant 0 \\ s_i - U(1 - y_i) \leqslant 0 \\ \sum y_i = n_{\boldsymbol{z}} + 1 \\ \boldsymbol{\theta}^{\mathrm{N}} - \delta\Delta\boldsymbol{\theta}^{-} \leqslant \boldsymbol{\theta} \leqslant \boldsymbol{\theta}^{\mathrm{N}} + \delta\Delta\theta^{+} \\ y_i = 0, 1; \quad \delta \geqslant 0; \quad \lambda_i \geqslant 0; \quad s_i \geqslant 0; \quad i \in I \end{cases} \tag{P1}$$

where $n_{\boldsymbol{z}}$ is the number of control variables of $\boldsymbol{z}$, $U$ represents an upper bound for the slacks. If $f_i = 0$, then $y_i = 1$, $s_i = 0$, which indicates constraint $i$ is active; if $f_i < 0$, then $y_i = 0$, which indicates constraint $i$ is inactive. The active constraint strategy suggests that $n_{\boldsymbol{z}} + 1$ constraints must be active for the final result. This conclusion is drawn from the fact that the largest $\boldsymbol{T}(\delta)$ is determined by the critical point which was the intersecting point of $\boldsymbol{T}(\delta)$ and $\boldsymbol{\Psi}(\boldsymbol{d}, \theta) = \boldsymbol{0}$, while $\boldsymbol{\Psi}(\boldsymbol{d}, \theta) = \boldsymbol{0}$ is just the projection result of a set of $n_{\boldsymbol{z}} + 1$ active constraints ($f_i = 0$). Note the subset of $n_{\boldsymbol{z}} + 1$ active constraints as $\overline{y}_k$ and the total candidate active sets as $\overline{Y}$, $\overline{y}_k \in \overline{Y}$. The active constraint strategy may be interpreted as follows: from one set of $\overline{y}_k$, a maximum $\delta_k$ could be obtained, then the flexibility index $F$ is the minimum one of all the possible $\delta_k$, *i.e.*, $F = \min_k \delta_k$. As the number of active constraint set is finite, the strategy is computationally efficient[9-11]. One visual representation of above discussion is shown in Fig. 2.

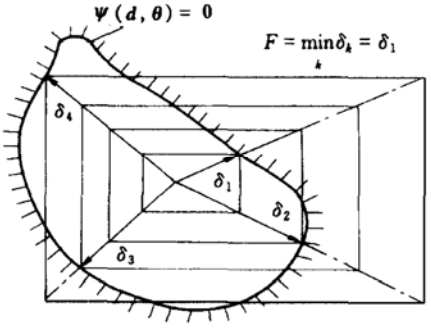


**Figure 2 Sketch for the active constraint strategy**

The hyperrectangle derived from the flexibility index F is similar with the initial hyperrectangle formed by a *priori* $\Delta\theta^{+}$, $\Delta\theta^{-}$ in $\theta$ space. It is the scalar F which dominates the expansion of all the dimensions of $\theta$. In the solution process, such cases always occur that when one vertex attained the feasible boundary all the other vertexes would correspondingly stop expanding even though they are still potentially extendible ( see Fig. 2 ). Thus, the hyperrectangle obtained with previous methods is rather conservative in most cases.

An important feature of the active constraint strategy is that the solution of P1 provides the positional information of critical point $\theta^{\mathrm{C}}$, which could be used to extend the other vertexes as farther as possible.

## 3 LOCAL ADJUSTING METHOD FOR MAXIMUM HYPERRECTANGLE

As discussed in the above, a local adjusting method for maximizing the hyperrectangle is proposed in this paper. Assuming the number of uncertain parameters are $NP$. The result of P1 may give the maximum hyperrectangle $T^1$ similar with the initial one, vertex of $\theta^{\mathrm{C}_1}$, scalar parameter $\delta^*$ and active constraint subset of $\overline{y}_1$. Here $\theta^{\mathrm{C}_1}$ determines the values of either $\theta_j^{+}$ or $\theta_j^{-}$ for all uncertain parameters $\theta_j (j = 1, \cdots, NP)$. We use two binary variables $\tau_j^{+}$, $\tau_j^{-}$ to indicate whether $\theta_j^{+}$ or $\theta_j^{-}$ is just decided.

$$\begin{cases} \text{If} \quad \theta_j^{+} \quad \text{fixed}, \tau_j^{+} = 1, \quad \text{otherwise} \quad \tau_j^{+} = 0 \\ \text{If} \quad \theta_j^{-} \quad \text{fixed}, \tau_j^{-} = 1, \quad \text{otherwise} \quad \tau_j^{-} = 0 \end{cases}$$

Then we reconfigure the hyperrectangle using the local adjusting method (LAM) as shown in Fig. 3

The proposed LAM method makes those undetermined $\theta_j^{+}$ or $\theta_j^{-}$ still have the possibility to extend as far as possible. After substituted back to P1, the reconfigured hyperrectangle generates the next new extended hyperrectangle $T^2$ with $\delta^*$, $\theta^{\mathrm{C}_2}$ and $\overline{y}_2$. Analogically, we can get the final and the largest hyperrectangle of the flexibility region.

## 4 EXTENDED ALGORITHM OF FLEXIBILITY ANALYSIS

Based on the proposed LAM, an extended algorithm is developed to find the largest flexibility hyperrectangle for a fixed chemical plant. The steps in this algorithm are as follows:

Step 1 Initialize the algorithm and set $\tau_j^{+} = 0$, $\tau_j^{-} = 0$, $k = 1$.

Step 2 Solve optimization problem P1 to yield the critical point $\theta^{\mathrm{C}}$, scalar parameter $\delta^*$ and active constraint subset $\overline{y}_k$.

Step 3 Generate the hyperrectangle according to current $\delta^*$, $\theta^{\mathrm{C}}$ and $\overline{y}_k$ with LAM method.

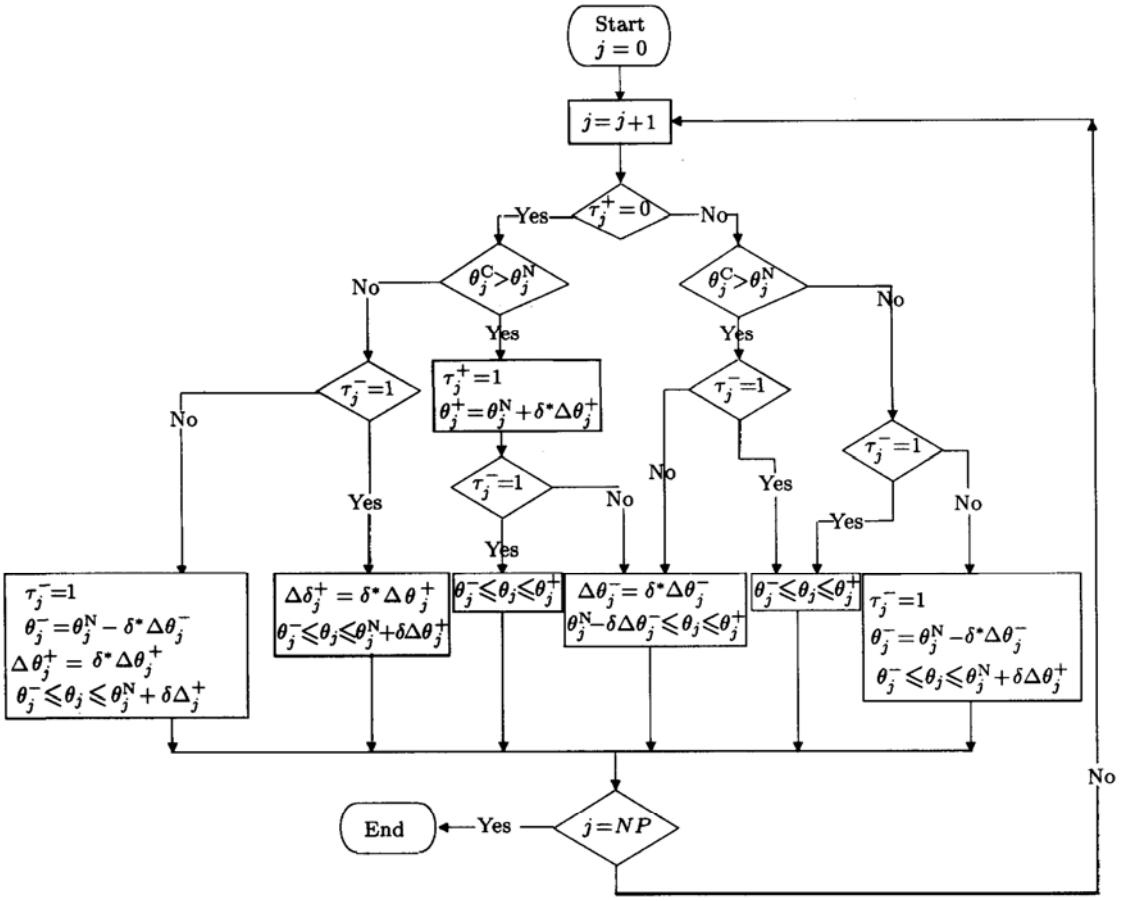


**Figure 3 Diagram of the local adjusting method**

Step 4 If $\sum_j \tau_j^+ + \tau_j^- = 2NP$, then Stop. Output the latest hyperrectangle. Otherwise, $k = k+1$, go to Step 5.

Step 5 Replace the hyperrectangle in problem P1 by the new one obtained in Step 3. Simultaneously, eliminate the $\overline{y}_k$ from the total candidate active sets $\overline{Y}$, then go to Step 2.

## 5 ILLUSTRATING EXAMPLES

The proposed algorithm is illustrated by two examples. Example 1 is a numerical one which involves the following set of four constraints with one control variable $z$ and two uncertain parameters $\theta_1$ and $\theta_2$

$$f_1 = z - \theta_1 + 2\theta_2 + d_1 - 3d_2 \leqslant 0$$
$$f_1 = -z - 0.5\theta_1 - \theta_2 + d_2 + 1 \leqslant 0$$
$$f_3 = z + \theta_1 - \theta_2 - d_1 - 8 \leqslant 0$$
$$f_4 = z + 2\theta_1 + 2\theta_2 - 2d_1 - 3d_2 \leqslant 0$$

The design values of $\boldsymbol{d}$, the nominal values and the expected deviations of $\boldsymbol{\theta}$ are given in Table 1. The boundary of the feasible region of example 1[$\Psi(\boldsymbol{d},\boldsymbol{\theta}) = \mathbf{0}$] can be obtained from the aboved 4 constraints (Fig. 4).

**Table 1 Data for example 1**

| $d_1$ | $d_2$ | $\theta_1^N$ | $\theta_2^N$ | $\Delta\theta_1^+$ | $\Delta\theta_1^-$ | $\Delta\theta_2^+$ | $\Delta\theta_2^+$ |
|---|---|---|---|---|---|---|---|
| 4 | 5 | 5 | 7 | 1 | 3 | 3 | 7 |

$$\Psi_1 = -1.5\theta_1 + \theta_2 - 5 = 0$$
$$\Psi_2 = 0.5\theta_1 - 2\theta_2 - 6 = 0$$
$$\Psi_3 = 1.5\theta_1 + \theta_2 - 17 = 0$$

By using the extended algorithm of flexibility analysis, the calculation results are obtained after 3 iterations as shown in Table 2. The extended hyperrectangles are shown in Fig. 5.

According to the iteration results, the final generated hyperrectangle is obviously much larger than the one calculated by previous method (iteration 1), which means the new algorithm fully exploits the flexibility region over which the feasible operation is guaranteed.

It should be noted that half of all the $2NP$ values of $\theta_j^+$ and $\theta_j^-$ are to be determined during the first iteration. Then at least one $\theta_j^+$ or $\theta_j^-$ will be determined for each following iteration so that when the new algorithm is completed at most $NP+1$ iterations are required.

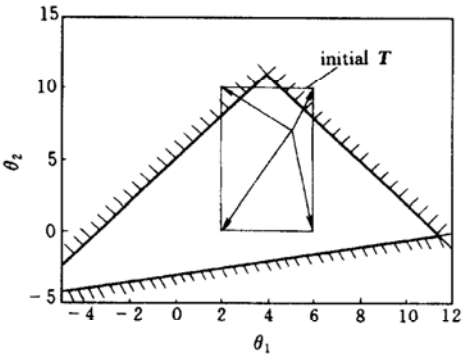


**Figure 4 Feasible region and initial $T$ in example 1**

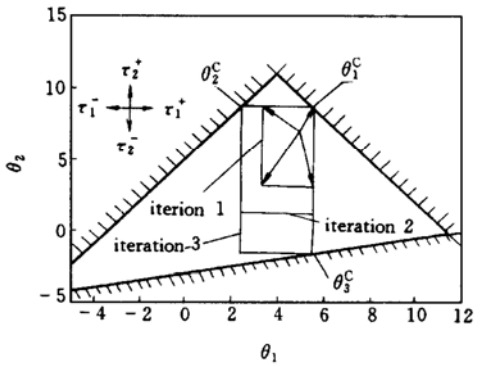


**Figure 5 Extending process in example 1**

Example 2 is an extended version of a practical chemical process given by Swaney[7]. In this example, a centrifugal pump (Fig. 6) transports liquid at a flowrate $m$ from its source at pressure $p_1$ through a pipe to its destination at pressure $p_2^*$. The flowrate $m$ and $p_2^*$ are treated as uncertain parameters $\theta$. The control variable is the valve coefficient $C_v$. The design variables $\boldsymbol{d}$, process constants, nominal values and the expected deviations for $\theta$ are shown in Table 3.

The reduced inequalities of $f_i(d, z, \theta) \leqslant 0$ for this example are given as follows

$$(p_1 + \rho H - \frac{m^2}{\rho C_v^2} - km^{1.84}D^{-5.16}) - p_2^* - \varepsilon \leqslant 0$$

$$-(p_1 + \rho H - \frac{m^2}{\rho C_v^2} - km^{1.84}D^{-5.16}) + p_2^* - \varepsilon \leqslant 0$$

$$mH - \eta W \leqslant 0$$

$$C_v - C_v^{MAX} \leqslant 0$$

$$rC_v^{MAX} - C_v \leqslant 0$$

The calculation results obtained by the proposed algorithm are shown in Table 4. And the extended hyperrectangles are shown in Fig. 7.

It should be pointed out that example 2 undergoes only two iterations before generating the final hyperrectangle, that is because $\theta_1^-$ and $\theta_2^-$, which were undetermined in the first iteration, are fixed synchronously in the second iteration (see Fig. 7). From the view of practical point, this coincidence occurs often, which means the actual iteration number of the proposed algorithm may be less than $NP + 1$.

**Table 2 Iteration results of example 1**

| Iteration | $\delta^*$ | $\theta_1^C$ | $\theta_2^C$ | $\tau_1^+$ | $\tau_1^-$ | $\tau_2^+$ | $\tau_2^-$ | $\overline{y}_k$ | Generated hyperrectangle |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 0.556 | 5.556 | 8.667 | 1 | 0 | 1 | 0 | $y_2 = 1, y_4 = 1$ | $3.332 \leqslant \theta_1 \leqslant 5.556$ |
| | | | | | | | | | $3.108 \leqslant \theta_2 \leqslant 8.667$ |
| 2 | 1.532 | 2.445 | 8.168 | 1 | 1 | 1 | 0 | $y_1 = 1, y_2 = 1$ | $2.445 \leqslant \theta_1 \leqslant 5.556$ |
| | | | | | | | | | $1.039 \leqslant \theta_2 \leqslant 8.667$ |
| 3 | 1.444 | 5.556 | 8.667 | 1 | 1 | 1 | 1 | $y_2 = 1, y_3 = 1$ | $2.445 \leqslant \theta_1 \leqslant 5.556$ |
| | | | | | | | | | $-1.661 \leqslant \theta_2 \leqslant 8.667$ |

**Table 3 Data for example 2**

| Design variables | Process constants | Values of uncertain parameters |
|---|---|---|
| driving power: $W = 35\,\mathrm{kW}$ | pump efficiency: $\eta = 0.5$ | desired pressure: $p_2^{*N} = 800\,\mathrm{kPa}$ |
| pump head: $H = 1.4\,\mathrm{kJ \cdot kg^{-1}}$ | control valve range: $r = 0.05$ | $\Delta\theta_1^+ = 200\,\mathrm{kPa}$ |
| pipe diameter: $D = 0.072\,\mathrm{m}$ | liquid density: $\rho = 1000\,\mathrm{kg \cdot m^{-3}}$ | $\Delta\theta_1^- = 550\,\mathrm{kPa}$ |
| control valve size: $C_v^{MAX} = 0.09$ | source pressure: $p_1 = 100\,\mathrm{kPa}$ | liquid flowrate: $m^N = 10\,\mathrm{m \cdot s^{-1}}$ |
| | pressure drop constant: $k = 9.101 \times 10^{-6}\,\mathrm{kPa}$ | $\Delta\theta_2^+ = 2\,\mathrm{kPa}$ |
| | tolerance of $p_2^*$: $\varepsilon = 20\,\mathrm{kPa}$ | $\Delta\theta_2^- = 5\,\mathrm{kPa}$ |

**Table 4 Iteration results of example 2**

| Iteration | $\delta^*$ | $\theta_1^C$ | $\theta_2^C$ | $\tau_1^+$ | $\tau_1^-$ | $\tau_2^+$ | $\tau_2^-$ | $\overline{y}$ | Generated hyperrectangle |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 0.535 | 906.650 | 11.067 | 1 | 0 | 1 | 0 | $y_2 = 1, y_4 = 1$ | $505.53 \leqslant \theta_1 \leqslant 906.650$ |
| | | | | | | | | | $7.323 \leqslant \theta_2 \leqslant 11.067$ |
| 2 | 1.929 | 232.461 | 4.841 | 1 | 1 | 1 | 1 | $y_2 = 1, y_5 = 1$ | $232.461 \leqslant \theta_1 \leqslant 906.650$ |
| | | | | | | | | | $4.841 \leqslant \theta_2 \leqslant 11.067$ |

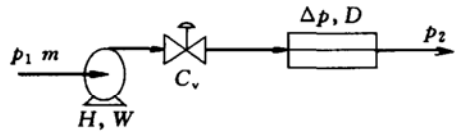


**Figure 6 Pump and system in example 2**

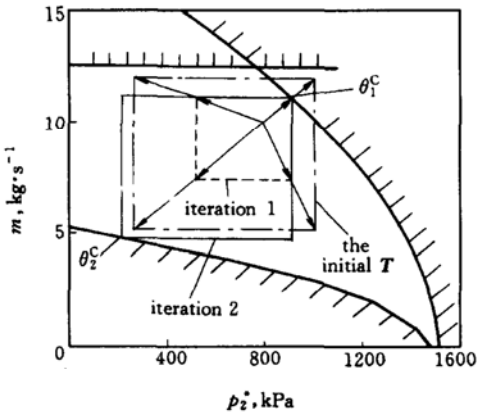


**Figure 7 Extending process for example 2**

For the higher dimensional uncertainty problems, which mean $n_{\mathbf{Z}} > 2$, the proposed extended algorithm is applicable in general. In fact, each iteration of the proposed algorithm would have fixed one of $\tau_j^+$ or $\tau_j^-$, which reduces the problem dimensionality. Therefore, higher dimensional problems would be transformed to lower dimensional ones during the iteration procedure, which shows the generality of the proposed algorithm.

## 6 LIMITATION OF THE EXTENDED ALGORITHM OF FLEXIBILITY ANALYSIS

The main limitation of the proposed algorithm is the assumption that the constraint functions $\boldsymbol{f}(\mathbf{d}, \boldsymbol{\theta}, \boldsymbol{z})$ should be jointly quasi-convex in $\boldsymbol{z}$ and one dimensional quasi-convex in $\boldsymbol{\theta}$[9], so that the critical point must lie at a vertex of the hyperrectangle. To practical chemical process it might be difficult to determine whether $\boldsymbol{f}(\mathbf{d}, \boldsymbol{\theta}, \boldsymbol{z})$ belongs to the functions described above. The following procedure could be used to check whether the final generated hyperrectangle is correct or not

$$\chi = \max_{\boldsymbol{\theta} \in \boldsymbol{T}^*} \min_{\boldsymbol{z}} \max_{i \in I} f_i(\boldsymbol{d}, \boldsymbol{z}, \boldsymbol{\theta})$$

$$\begin{cases} \text{if} \quad \chi \leqslant 0 & \text{all the constraints are satisfied,} \\ & \text{the result is correct} \\ \text{if} \quad \chi > 0 & \text{some constraints are not satisfied,} \\ & \text{the result is incorrect} \end{cases} \tag{8}$$

The above problem can also be solved with the active constraint strategy,

$$\chi = \max_{\boldsymbol{\theta}, \boldsymbol{z}, u, S_i, \lambda_i, y_i} u$$

s.t.

$$\begin{cases} f_1(\boldsymbol{d}, \boldsymbol{z}, \boldsymbol{\theta}) - u + s_i = 0 \\ \sum_i \lambda_i = 1 \\ \sum_i \lambda_i \dfrac{\partial f_i}{\partial \boldsymbol{z}} = 0 \\ \lambda - y_i \leqslant 0 \\ s_i - U(1-y)i) \leqslant 0 \\ \sum y_i = n_{\boldsymbol{z}} + 1 \\ \boldsymbol{T}^* = \left\{ \boldsymbol{\theta} \middle| \boldsymbol{\theta}^{\mathrm{L}} \leqslant \boldsymbol{\theta} \leqslant \boldsymbol{\theta}^{\mathrm{U}} \right\} \\ y_i = 0, 1; \lambda_i \geqslant 0; s_i \geqslant 0; i \in I \end{cases} \tag{P2}$$

where $\boldsymbol{T}^* = \left\{ \boldsymbol{\theta} \middle| \boldsymbol{\theta}^{\mathrm{L}} \leqslant \boldsymbol{\theta} \leqslant \boldsymbol{\theta}^{\mathrm{U}} \right\}$ is the final hyperrectangle generated by the proposed algorithm. $\theta^{\mathrm{L}}$, $\theta^{\mathrm{U}}$ are the lower and upper bounds of the final uncertainties of $\theta$, respectively.

For example 2, $\chi = -0.71 \times 10^{-4}$ is obtained. From Eq. (8) it is shown that the extended hyperrectangle is feasible for the practical chemical process.

The same result by previous methods is obtained in the first iteration of the proposed extended algorithm. From then on, the subsequent iteration would generate a larger hyperrectangle than before. Even if the results are incorrect due to the convexity limitation of the constraint functions, they could be effectively detected and removed by the proposed check procedure. Therebefore, the final hyperrectangle generated by the proposed algorithm would be larger than the one obtained with previous methods.

## 7 CONCLUSIONS

The proposed LAM method and extended algorithm of flexibility analysis exploits the flexibility region over which a chemical process could hold the feasible operation. With the LAM method, the active constraint strategy is used repeatedly to obtained a series of critical points of $\theta^{\mathrm{C}}$, in the meantime the hyperrectangle of uncertainty space is extended effectively. The hyperrectangular flexibility region generated by the extended algorithm will be larger than that obtained with previous methods. The limitation of the proposed algorithm due to imperfect convexity is discussed and its corresponding verification measure is confirmed to be effective. The proposed new algorithm is proved useful for flexibility analysis of practical chemical process design and operation.

## NOMENCLATURE

| | |
|---|---|
| $\boldsymbol{d}$ | vector of design variables |
| $F$ | flexibility index |
| $NP$ | number of uncertain parameters |

| | |
|---|---|
| $n_{\boldsymbol{z}}$ | number of control variables of $\boldsymbol{z}$ |
| $\boldsymbol{S}$ | vector of slack variables |
| $\boldsymbol{T}$ | hyperrectangle for uncertain parameters |
| $\boldsymbol{T}(\delta)$ | hyperrectangle with scalar variable $\delta$ |
| $U$ | upper bound for the slack variables |
| $u$ | scalar for maximum constraint value |
| $\boldsymbol{x}$ | vector of state variables |
| $\overline{Y}$ | total candidate of $\overline{y}$ |
| $\overline{y}$ | active subset for $y_i$ |
| $y_i$ | binary variable for constraint $i$ |
| $\boldsymbol{z}$ | vector of control variables |
| $\delta$ | scaled parameter deviation |
| $\boldsymbol{\theta}$ | vector of uncertain parameters |
| $\boldsymbol{\theta}^{\mathrm{C}}$ | critical point of vector $\boldsymbol{\theta}$ |
| $\boldsymbol{\theta}^{\mathrm{N}}$ | nominal point of vector $\boldsymbol{\theta}$ |
| $\Delta\boldsymbol{\theta}^{+}$ | positive deviation of vector $\boldsymbol{\theta}$ |
| $\Delta\boldsymbol{\theta}^{-}$ | negative deviation of vector $\boldsymbol{\theta}$ |
| $\theta_j^{+}$ | upper bound for $\theta_j$ |
| $\theta_j^{-}$ | lower bound for $\theta_j$ |
| $\boldsymbol{\lambda}$ | vector of Lagrange multipliers |
| $\tau_j^{+}$ | director factors for $\theta_j^{+}$ |
| $\tau_j^{-}$ | director factors for $\theta_j^{-}$ |
| $\boldsymbol{\Psi}$ | feasible function |

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