Procedure for Improving Dynamic Operability of Chemical Processes

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Abstract A simple and effective method for improving Euclidean norm condition number for chemical processing system is presented. The singular value sensitivities of Freudenberg *et al.* (1982) is used to estimate the behavior of singular values of process transfer function matrix when design parameter is changed, then the condition number can be calculated straightforwardly. The method requires explicit dependencies of each transfer function matrix elements on design parameters. These dependencies can be obtained either by symbolic differentiation in the form of explicit function of design parameters, or by numerical perturbation studies for units with large and complicated models. Gerschgorin-type lower bound for minimum singular value is introduced to detect the large divergencies near singular point due to linearity of sensitivities. The case studies are performed to show the efficiency of the proposed method.

Keywords Controllability, Condition Number, Singular Value Analysis, Process Design, Sensitivity Analysis

1. Introduction

Chemical processes are subject to various uncertainties during operations. Controllability is an ability of process to operate economically and safely - without violating constraints - to achieve various design objectives in the presence of theses uncertainties. Many works have been done to develop the controllability assessment technique, but, the methods for designing process with better controllability or improving it lack in literatures (Morari 1994).

Since controllability is an inherent property of process itself, one should consider it at the design stage before control system is fixed. The most preferable way to consider controllability at the design stage is to include controllability as one of the design objectives just like traditional economic ones in design optimization problem. Unfortunately, many controllability assessment methods and indices are based on and defined in different domains from those of design problems.

In this study, we developed the method for incorporating resilience index as one of various objectives in process design optimization problem. Among many controllability assessment techniques, condition number, which measures resilience of process, is adopted as the index to be improved.

2. Singular Value Analysis

Condition number quantifies robustness of process in the presence of the model mismatch to real process. It is defined as the ratio of maximum and minimum singular values of process transfer function matrix. In MIMO (Multi-Input Multi-Output) case, the gain of process is variable with respect to magnitudes and directions of input vectors. Singular value analysis can provide valuable information about these MIMO gains.

For arbitrary complex matrix $A \in C_r^{m\times n}$, there exist orthogonal pair of matrix $U \in C_r^{m\times m}$ and $V \in C_r^{n\times n}$, which satisfy following relations.

$$A = U \Sigma V^T \qquad (1)$$

Where, T means complex conjugate transpose, and matrix U and V are unitary ($U^T = U^{-1}$). Σ is diagonal matrix whose elements are ordered as follows.

$$\Sigma = diag(\sigma_1, \sigma_2, \cdots, \sigma_r) \qquad (2)$$

Where, r is a rank of matrix A, and elements of set $\{\sigma_i\}$ are singular values. Singular values are square roots of eigenvalues of matrix $A^T A$, with a order of

$$\sigma_1 \ge \sigma_2 \ge \cdots \ge \sigma_r \ge 0 \qquad (3)$$

Practically, the largest singular value of process transfer matrix G means the upper limit of the ratio of response of G to sinusoidal input. If a process has a large condition number, response will vary in large amount according to direction and magnitude of input, and becomes very difficult to predict the response with model even with small amount of error with real process. Therefore, the lower the value of condition number, it is easier to design and install the control system which can successfully deal with various input changes regardless of model mismatch or manipulated variable constraints exist. Singular value analysis also quantifies the effect of manipulated variables constraints on controllability.

There are some very useful properties of singular value analysis.

$$\begin{aligned} Av_j &= \sigma_j(G)\,u_j \\ Av_{\max} &= \sigma_{\max}(G)\,u_{\max} \\ Av_{\min} &= \sigma_{\min}(G)\,u_{\min} \end{aligned} \qquad (4)$$

$u_{\min}(G)$ is input or disturbance which generates minimum amplification, and $u_{\max}(G)$ maximum.

If the condition number is large, the difference of controller gains necessary to compensate the undesirable process responses due to given disturbances in the direction of maximum and minimum amplifications is very large, and it becomes difficult to design such a controller.

3. Incorporating Condition Number in Process Design

Various process design activities are carried out based on process models with various levels of complexities and abstractions. Primarily, chemical and physical principles comprise those models. The one of the most common and important objective in process design is economics, and this requires design parameters as a variables for their function. Unfortunately, the condition number of chemical process is calculated numerically from process transfer function matrix, and it is difficult to establish the effect of design parameters to condition number intuitively. Therefore it is highly required to find the method for relating condition numbers and design parameters so as to integrate the controllability aspect in whole design optimization problem.

Condition number of a matrix is defined as a ratio of maximum and minimum singular values, and is very difficult to derive analytical function of each element of matrix even

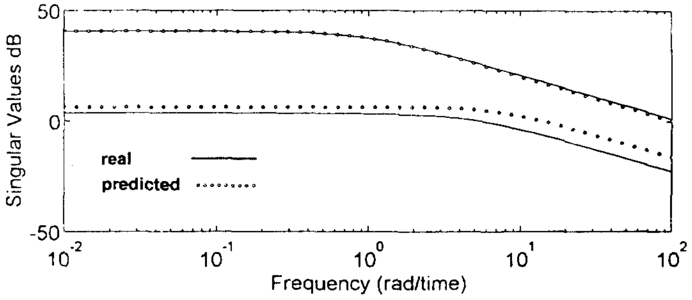

Fig. 1. Real and estimated singular values.

the size of matrix is small, say 2×2. Furthermore, it is impossible to derive such an analytic equations for matrix larger than 3×3.

To overcome this difficulty, we introduce the singular value sensitivities of Freundenberg *et al.* (1982) which is defined as follows. The frequency dependency terms are dropped for convenience.

$$\nabla\sigma_i(p;\Delta p) \;=\; Re\;\left[u_i(p)^T\delta G(p;\Delta p)v_i(p)\right] \qquad (5)$$

$$\textit{where,}\quad \delta G(p;\Delta p) = \sum_{i=1}^{m}\nabla_i G(p)\Delta p_i$$
$$Re\,[M] = \frac{1}{2}\,[M+M^T]$$

Basically, process transfer function matrix can be attained from analytic derivation - in case of very simple model - or from numerical perturbation studies by simulation. The above mentioned sensitivities then can be derived respect to design parameters. Fig. 1. compares the real and estimated values of condition number of following transfer matrix, whose elements are given as an analytic function of a design parameter p.

$$G(s) = \begin{pmatrix} \dfrac{16.9(1+\Delta p^2)}{(s+5)} & \dfrac{36.12(2\Delta p+1)}{(s+1)} \\ \dfrac{-9.57(2-\Delta p)}{(s+5)} & \dfrac{-4.17(1+\Delta p/2)}{(s+1)} \end{pmatrix}$$

The sensitivities can be easily calculated by commercial matrix calculation packages such as MATLAB®. As shown in Fig. 1., the estimated singular values by sensitivities predict real values quite well with acceptable errors.

Since the sensitivities of each singular values to design parameter changes are given as constant value, it becomes very easy to incorporate the dependencies of condition number in process design optimization problem as one of

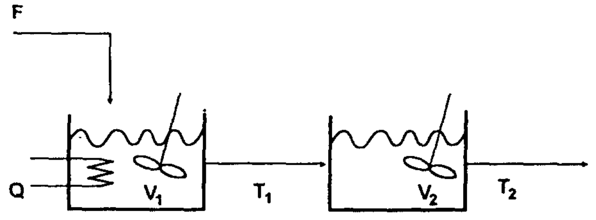

Fig. 2. Two-stage heating tank example.

the objective functions. However, the limit of constant dependencies - linearities - can forces us to introduce additional consideration which will be described in following section.

4. Gerschgorin-type Bounds

Singular value estimation based on sensitivities is basically linear. Therefore, it is not recommended to use this method for wide range of design parameter changes without any modification. Estimation error becomes more larger when the transfer function matrix moves to near singular point region. At singular point, the minimum singular value becomes zero and the rank of the matrix is reduced - the number of non-zero singular values equals to the rank of matrix. Thus the process near singular point tends to have a extremely large condition number due to very small minimum singular value. The estimation of minimum singular value gives impossible negative value at singular point.

Thus we introduced Gerschgorin-type lower limit for minimum singular value. This monitoring criteria is little conservative, but tight enough to detect large error occurred due to high nonlinearities or singular point. It only requires the elements of matrix, hence, easily integrated in optimization formulation for process design. If the estimated singular values violate the introduced lower limit, sensitivities should be recalculated at that point. Generally, design near singular point should be avoided, the precise value of minimum singular value is not necessary, and the Gerschgorin-type lower limit can afford us enough information to avoid the direction of design modification which leads to near singular point region.

Gerschgorin theorem is originally for the approximation of

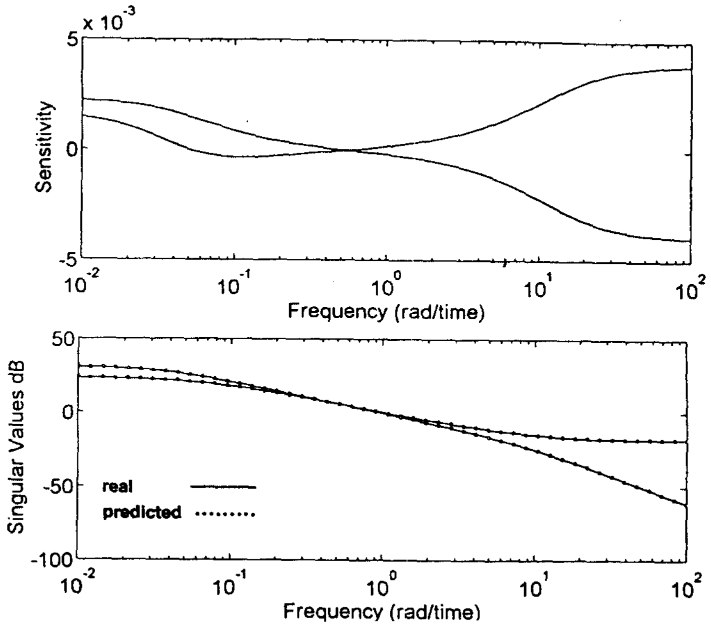

Fig. 3. Effect of change in V_1.

eigenvalues of matrix as follows.

Theorem 1. All eigenvalues of matrix A is located within the union of Gerschgorin disks. Where Gerschgorin disk is defined as follows.

$$|\lambda - a_{ii}| \le r'_i, \quad i = 1,2,\cdots,n \qquad (6)$$

$$\text{where,} \quad r_i = |a_{i1}| + |a_{i2}| + \cdots + |a_{in}| = \sum_{k=1}^{n} |a_{ik}|$$

$$r'_i = r_i - |a_{ii}|$$

Proof see Goldberg (1992) ■

From this theorem, it is straightforward to derive the approximated limit of singular value of a matrix. In this study, we adopted following improved equation of Hong and Pan (1992).

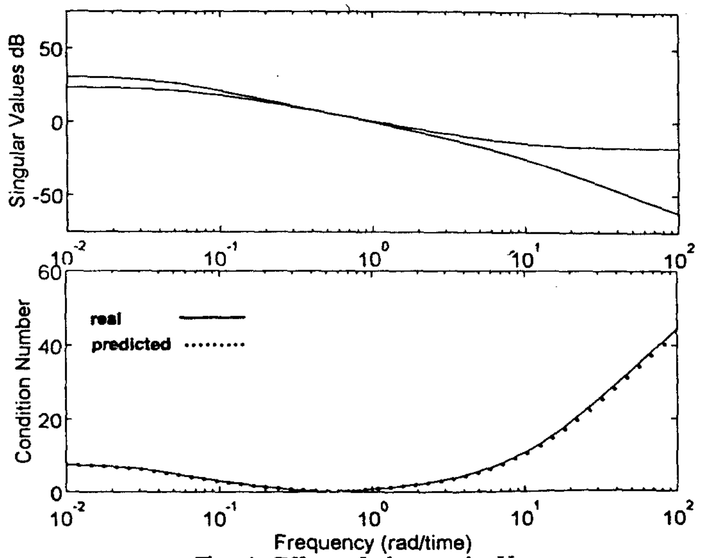

Fig. 4. Effect of changes in V_2

$$\sigma_{\min}(A) \geq \left(\frac{n-1}{n}\right)^{(n-1)/2} |A| \max\left\{\frac{c_{\min}(A)}{\prod_{i=1}^{n} c_i(A)}, \frac{r_{\min}(A)}{\prod_{i=1}^{n} r_i(A)}\right\} \quad (8)$$

5. Example

Case study is performed to demonstrate the efficiency of the proposed procedure. The schematics of the example process is shown in Fig. 2. The process is two serially connected heating tanks and can be described by following state-space models. Detailed descriptions data can be found in Kwon (1995).

$$A = \begin{pmatrix} \frac{-F_s}{V_1} & 0 \\ \frac{F_s}{V_2} & \frac{-F_s}{V_2} \end{pmatrix}$$

$$B = \begin{pmatrix} \frac{1}{V_1 c_p} & \frac{(T_0 - T_{1s})}{V_2 c_p} \\ 0 & 0 \end{pmatrix}$$

$$C = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Then the process transfer function matrix can be easily obtained from following relation.

$$G = C(sI - A)^{-1}B \quad (7)$$

For the illustration purpose, V_1 and V_2 are selected as design parameters. Fig. 3. and Fig. 4. shows the sensitivities of maximum and minimum singular values to each design parameters. Then, the simple LP problem can be formulated to find the optimum design change to attain desired condition number value at considered range of frequencies with minimum cost for design modification.

6. Conclusion

A simple and effective method to incorporate condition number as a objective function of process design is proposed. The singular value sensitivities are introduced to estimate the effect of changes of design parameters on condition numbers. In order to integrate condition number into the framework of conventional design optimization, sensitivity of condition number to design parameters is employed and Gerschgorin-type bounds are used to overcome the inaccuracy from linear assumption. Although the method is not rigorous, it gives valuable information to enhance controllability of chemical processes.

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References

Freudenberg J.S., Looze, D.P. and Cruz, J.B. 1982. Robustness Analysis using Singular Value Sensitivities. Int. J. Control, 35(1), 95~116

Goldberg, J.L. 1992. Matrix Theory with Applications, McGraw-Hill, New York

Hong, Y.P. and Pan, C.T. 1992. A Lower Bound for the Smallest Singular Value. Linear Algebra and Its Applications, 172, 27~32

Kwon, Y.W. 1995. A Study on Improving Dynamic Operability of Chemical Processes Based on Structural Analysis and Quantitative Controllability Measures, Ph.D. Thesis, Seoul National University

Morari, M. 1992. Effect of Design on the Controllability of Continuous Plants, Proceedings of Interactions between Process Design and Process Control, 3~16