QUANTITATIVE ANALYSIS OF THE SAFETY AND FLEXIBILITY OF NONLINEAR DYNAMIC SYSTEMS

H. Huang, C. S. Adjiman*, N. Shah
Centre for Process Systems Engineering
Department of Chemical Engineering and Chemical Technology
Imperial College of Science, Technology and Medicine
Prince Consort Road, London SW7 2BY, U.K.

Abstract

We present a methodology to identify safe or feasible operating regions in the space of some of the key operational variables and unknown parameters for processes described by nonlinear dynamic or algebraic equations. A feasibility test is performed by combining a monotonicity analysis of the algebraic or discretized dynamic model with interval arithmetic tools. This approach is used within a branch-and-bound approach to identify the possibly nonconvex boundary between feasible and infeasible regions and determine the overall size of the feasible region. This approach is applied to three case studies.

Keywords

Flexibility analysis, Nonconvex feasible region, Interval arithmetic

Introduction

Flexibility is a key issue in the design and operation of chemical processes. Halemane and Grossmann (1983) introduced the feasibility test and defined a max-min-max problem which can be solved rigorously for quasi-convex problems. Swaney and Grossmann (1985) then developed the flexibility index problem to identify the largest hyper-rectangle that can be inscribed in the feasible region around a nominal point. Floudas and Grossmann (1987) proposed an active set strategy to solve the problem. Dimitriadis and Pistikopoulos (1995) extended the approach to deal with dynamic systems. Recently, Samsatli et al. (2001) proposed an approach which does not rely on a nominal operating point but which still restricts the region of interest to a hyper-rectangular shape. Ierapetritou (2001) proposed a methodology which can inscribe a polygon in a convex feasible region. Adjiman (1999) and Huang et al. (2002) considered the identification of safe operating regions for nonlinear dynamic open-loop systems, using interval arithmetic (Moore, 1979) and monotonicity analysis within a branch-and-bound framework. This approach deals with nonconvex feasible or safe regions in the space of uncertainties.

In this paper, we extend this work to deal with systems with closed-loop control. Flexibility is defined as the ability of the process to maintain feasible operation over the time horizon (or at steady-state if dynamics are not considered) given uncertain operating conditions. We first present the general problem formulation. We then describe the algorithm used to tackle the problem. Finally, we apply the proposed methodology to three case studies.

Problem Formulation

We consider a general process model given by

$$\begin{aligned} &\boldsymbol{h}(\boldsymbol{x}, \dot{\boldsymbol{x}}, \boldsymbol{y}, \boldsymbol{z}, \boldsymbol{\theta}) = \boldsymbol{0} \\ &\boldsymbol{x}(0) = \boldsymbol{x}_0(\boldsymbol{\theta}) \end{aligned} \quad (1)$$

* To whom all correspondence should be addressed.

where $\boldsymbol{x}$ is an n-dimensional vector of time-dependent state variables, $\dot{\boldsymbol{x}}$ is the vector of time derivatives of $\boldsymbol{x}$, $\boldsymbol{y}$ is a p-dimensional vector of time independent variables, $\boldsymbol{z}$ is the q-dimensional vector of time-dependent control variables and θ is an m-dimensional vector of uncertain parameters. These include model parameters, varying inputs and operational degrees of freedom. $\boldsymbol{h}$ is an $n+p$-dimensional vector of equality constraints. The initial conditions can be a function of the uncertain parameters. The feasibility or safety of the process is ensured when inequality constraints on the performance or state of the process are met

$$\boldsymbol{g}\left(\boldsymbol{x},\dot{\boldsymbol{x}},\boldsymbol{y},z,\theta\right) \le \boldsymbol{0} \tag{2}$$

where $\boldsymbol{g}$ is a t-dimensional vector. It is assumed that both $\boldsymbol{h}$ and $\boldsymbol{g}$ are once continuously differentiable with respect to the variables. A feasible point is defined as a point θ^* such that there exists a control $\boldsymbol{z}^*$ such that at every time point Eqs (1) and (2) are satisfied.

Given a range $[\theta^L,\theta^U]$ for the uncertain parameters such that $\theta^L \le \theta \le \theta^U$, we define the feasible region $\mathcal{R}_F$ as the set of feasible points in $[\theta^L,\theta^U]$ and the infeasible region $\mathcal{R}_I$ as the set of points in $[\theta^L,\theta^U]\backslash\mathcal{R}_F$. We use a flexibility index F similar to that defined by Ierapetritou (2001)

$$F = \frac{V_F}{V_\theta} \tag{3}$$

where V_F is the volume of the feasible region within the uncertainty space $[\theta^L,\theta^U]$, and V_θ is the volume of the uncertainty space. In practice, we aim to calculate tight lower and upper bounds on F. This is achieved by building an approximation R_F to the feasible region such that $R_F \subseteq \mathcal{R}_F$ and an approximation R_I to the infeasible region such that $R_I \subseteq \mathcal{R}_I$. Then, we have

$$\frac{vol(R_F)}{vol([\theta^L,\theta^U])} \le F \le \frac{vol([\theta^L,\theta^U]\setminus R_I)}{vol([\theta^L,\theta^U])} \tag{4}$$

where $vol()$ denotes a function used to calculate the volume of an m-dimensional region.

Proposed Methodology

The feasibility test problem for a chemical process described by a dynamic model is given by (Dimitriadis and Pistikopoulos, 1995)

$$\chi = \begin{cases} \max\limits_{\theta} \min\limits_{z} \max\limits_{u} u \\ s.t. \quad \boldsymbol{g}(\boldsymbol{x},\dot{\boldsymbol{x}},\boldsymbol{y},z,\theta) \le u \\ \qquad \boldsymbol{h}(\boldsymbol{x},\dot{\boldsymbol{x}},\boldsymbol{y},z,\theta) = \boldsymbol{0} \\ \qquad \theta \in [\theta^L,\theta^U] \end{cases} \tag{5}$$

The proposed approach for the calculation of the bounds on F requires three main steps:

(i) the construction of upper and lower bounds on the solution of the feasibility test problem (5) for a given range of the uncertain parameters.
(ii) the use of a branch-and-bound algorithm to identify subregions R_F and R_I of the uncertainty space.
(iii) the calculation of the volume of lower and upper approximations to the feasible and infeasible regions.

An upper bound χ^{U*} on the solution of the feasibility test problem is obtained by solving the following optimization problem, as adapted from Ostrovsky et al. (2000)

$$\chi^{U*} = \begin{cases} \min\limits_{u} \max\limits_{\theta} u \\ s.t. \quad \boldsymbol{g}(\boldsymbol{x},\dot{\boldsymbol{x}},\boldsymbol{y},z,\theta) \le u \\ \qquad \boldsymbol{h}(\boldsymbol{x},\dot{\boldsymbol{x}},\boldsymbol{y},z,\theta) = \boldsymbol{0} \\ \qquad \theta \in [\theta^L,\theta^U] \end{cases} \tag{6}$$

A lower bound χ^{L*} on the solution of the feasibility test problem is obtained by solving the following problem

$$\chi^{L*} = \begin{cases} \min\limits_{u,\theta} u \\ s.t. \quad \boldsymbol{g}(\boldsymbol{x},\dot{\boldsymbol{x}},\boldsymbol{y},z,\theta) \le u \\ \qquad \boldsymbol{h}(\boldsymbol{x},\dot{\boldsymbol{x}},\boldsymbol{y},z,\theta) = \boldsymbol{0} \\ \qquad \theta \in [\theta^L,\theta^U] \end{cases} \tag{7}$$

To obtain rigorously valid bounds, problems (6) and (7) should be solved to global optimality. This difficult task can be avoided by building linear or convex relaxations of these two problems which can be solved to global optimality. This can be achieved by using the Region-Transition Model framework of Adjiman (1999) and Huang et al. (2002) in which Eqs. (1) and (2) are used to build a "bounding model" of the form

$$\begin{aligned} &\underline{\boldsymbol{h}}(\underline{\boldsymbol{x}},\overline{\boldsymbol{x}},\underline{\dot{\boldsymbol{x}}},\overline{\dot{\boldsymbol{x}}},\underline{\boldsymbol{y}},\overline{\boldsymbol{y}},z,\theta^L,\theta^U) = \boldsymbol{0} \\ &\overline{\boldsymbol{h}}(\underline{\boldsymbol{x}},\overline{\boldsymbol{x}},\underline{\dot{\boldsymbol{x}}},\overline{\dot{\boldsymbol{x}}},\underline{\boldsymbol{y}},\overline{\boldsymbol{y}},z,\theta^L,\theta^U) = \boldsymbol{0} \\ &\underline{\boldsymbol{g}} = \underline{\boldsymbol{g}}(\underline{\boldsymbol{x}},\overline{\boldsymbol{x}},\underline{\dot{\boldsymbol{x}}},\overline{\dot{\boldsymbol{x}}},\underline{\boldsymbol{y}},\overline{\boldsymbol{y}},z,\theta^L,\theta^U) \\ &\overline{\boldsymbol{g}} = \overline{\boldsymbol{g}}(\underline{\boldsymbol{x}},\overline{\boldsymbol{x}},\underline{\dot{\boldsymbol{x}}},\overline{\dot{\boldsymbol{x}}},\underline{\boldsymbol{y}},\overline{\boldsymbol{y}},z,\theta^L,\theta^U) \end{aligned} \tag{8}$$

where _ denotes a lower bound and ¯ denotes an upper bound. $\underline{\boldsymbol{h}} = \boldsymbol{0}$ and $\overline{\boldsymbol{h}} = \boldsymbol{0}$ are bounding equations which allow the derivation of bounds on the state variables, their derivatives and the time-independent variables. These bounding equations can be obtained by applying concepts from interval arithmetic (Moore, 1979), performing a monotonicity analysis of the model, and using physical bounds. Similarly, $\underline{g}$ and $\overline{g}$ are bounds on Eq. (2). We can then formulate the following two problems:

$$\chi^U = \begin{cases} \min_u u \\ s.t. \quad \overline{g}(\underline{x},\overline{x},\underline{\dot{x}},\overline{\dot{x}},\underline{y},\overline{y},z,\theta^L,\theta^U) \le u \\ \quad\quad \underline{h}(\underline{x},\overline{x},\underline{\dot{x}},\overline{\dot{x}},\underline{y},\overline{y},z,\theta^L,\theta^U) = 0 \\ \quad\quad \overline{h}(\underline{x},\overline{x},\underline{\dot{x}},\overline{\dot{x}},\underline{y},\overline{y},z,\theta^L,\theta^U) = 0 \end{cases} \quad (9)$$

$$\chi^L = \begin{cases} \min_u u \\ s.t. \quad \underline{g}(\underline{x},\overline{x},\underline{\dot{x}},\overline{\dot{x}},\underline{y},\overline{y},z,\theta^L,\theta^U) \le u \\ \quad\quad \underline{h}(\underline{x},\overline{x},\underline{\dot{x}},\overline{\dot{x}},\underline{y},\overline{y},z,\theta^L,\theta^U) = 0 \\ \quad\quad \overline{h}(\underline{x},\overline{x},\underline{\dot{x}},\overline{\dot{x}},\underline{y},\overline{y},z,\theta^L,\theta^U) = 0 \end{cases} \quad (10)$$

By construction, $\chi^L \le \chi^{L*} \le \chi \le \chi^{U*} \le \chi^U$. Thus, for a given uncertainty region $[\theta^L, \theta^U]$, the following feasibility test can be applied:

- If $\chi^U \le 0$, the region is *feasible*.
- If $\chi^L \ge 0$, the region is *infeasible*.
- Otherwise, the feasibility of the region is not determined.

One of the key properties of the Region Transition Model used is that as the size of the uncertainty region becomes smaller, its solution converges to the solution of model (1). As a result, the two bounds χ^L and χ^U also converge to χ in the limit of infinitesimally small uncertainty regions. This property can be exploited in a branch-and-bound algorithm as follows:

Step 1. Set initial region $R_0=[\theta^L, \theta^U]$. Set stacks $R_F=\varnothing$, $R_I=\varnothing$. Set working stack $R=\{R_0\}$. Set convergence tolerance ε. Set iteration counter k=0.
Step 2. If $R=\varnothing$, terminate. Else, remove a region R^k from R.
Step 3. Perform feasibility test on R^k.
Step 4. If R^k is feasible, add R^k to R_F. If it is infeasible, add R^k to R_I. Otherwise, if size(R^k)≤ε, discard R^k. Else, bisect R^k into two child regions and add child regions to R.
Step 5. Set $k=k+1$.

When the algorithm terminates, the two stacks R_F and R_I contain hyperrectangles whose volume can be readily calculated. This is then used to compute bounds on F.

Case Studies

We apply the proposed methodology to three case studies: the first is a simple linear algebraic heat exchanger example, the second a nonconvex algebraic example and the third a pseudo-dynamic heat exchanger network example.

Case Study 1

This simple example is taken from Biegler et al. (1997, pp 691-697). The feasibility constraints for this system can be expressed as a function of the uncertain parameters (T_3∈[325K, 450K] and T_4∈[500K, 650K]) and the control variable (Q_c) exclusively. Problems (9) and (10) are constructed by applying interval arithmetic to the feasibility constraints. This model is not shown here due to space limitations. The proposed algorithm is run with a convergence tolerance of 0.1 to obtain the results shown in Figure 1. A flexibility index of 0.519≤F≤0.521 is found. The feasible region obtained is the upper region delimited by three linear constraints. In this case, these constraints can also be derived analytically, yielding a flexibility index of 0.520. Using classical flexibility analysis and a nominal point (T_3^N, T_5^N)=(388,583), the shaded feasible region shown is obtained, giving a flexibility index of 0.050.

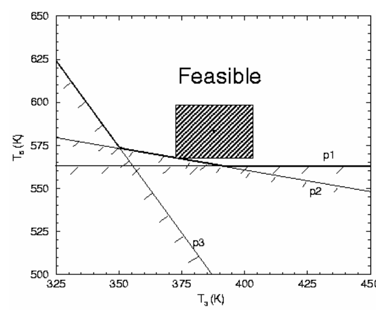

Fig. 1 –Flexibility analysis for Case study 1.

Case study 2

The second case study is a modified version of the example proposed by Ierapetritou (2001) in which the feasible region has been made nonconvex (see Fig. 2).

There are two uncertain parameters, θ_1∈[-5.0,5.0] and θ_2∈[-40.0,40.0]. The feasible region is described by

$$\begin{aligned} g_1 &= \theta_2 - (\theta_1 - 2)^2 - 20 \le 0 \\ g_2 &= (\theta_1 + 0.5)^2 - \theta_2 - 2.25 \le 0 \\ g_3 &= \theta_2 - 4\theta_1 - 30 \le 0 \end{aligned} \quad (11)$$

The upper and lower bounding functions for these constraints are respectively

$$\begin{aligned} \underline{g}_1 &= \underline{\theta}_2 - \max\left\{(\underline{\theta}_1 - 2)^2, (\overline{\theta}_1 - 2)^2\right\} - 20 \le 0 \\ \underline{g}_2 &= \min\left\{0, (\underline{\theta}_1 + 0.5)^2, (\overline{\theta}_1 + 0.5)^2\right\} - \overline{\theta}_2 - 2.25 \le 0 \\ \underline{g}_3 &= \underline{\theta}_2 - 4\overline{\theta}_1 - 30 \le 0 \end{aligned} \quad (12)$$

and

$$\overline{g}_1 = \overline{\theta}_2 - \min\left\{0, (\underline{\theta}_1 - 2)^2, (\overline{\theta}_1 - 2)^2\right\} - 20 \le 0$$
$$\overline{g}_2 = \max\left\{(\underline{\theta}_1 + 0.5)^2, (\overline{\theta}_1 + 0.5)^2\right\} - \underline{\theta}_2 - 2.25 \le 0$$
$$\overline{g}_3 = \overline{\theta}_2 - 4\underline{\theta}_1 - 30 \le 0 \tag{13}$$

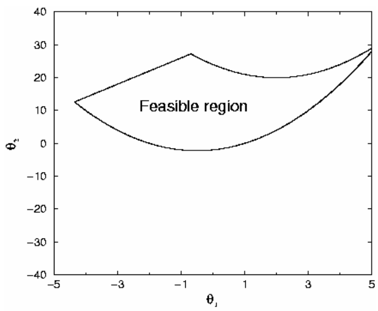

Fig. 2 – Feasible region for case study 2.

The application of the proposed methodology with ε=0.01 to this problem yields a highly accurate identification of the nonconvex boundary between the feasible and infeasible regions and determines that the system has a flexibility index such that $0.185 \le F \le 0.186$.

Case Study 3

The final example is a pseudo-dynamic case study taken from Dimitriadis and Pistikopoulos (1995). A heat exchanger network in which the heat transfer coefficient decays with time is considered. Here, only one of the heat exchangers can be bypassed. The uncertainty space is described by the inlet temperature of cold stream 1 ($T_{C1} \in [13,60]$) and the heat-capacity flowrate of hot stream 1 ($F_{H1} \in [20,60]$). The bounding model is constructed by using interval analysis and monotocity analysis, that is, determining the sign of the derivatives of the model variables with respect to the uncertain parameters. In this example, the time dependence can be handled in a straightforward manner, by noting that the worst-case scenario occurs at the final time, when the heat transfer coefficient is at its minimum value. The application of the proposed algorithm to this problem yields the results shown in Figure 3 with a nonconvex feasible region. The flexibility index is such that $0.207 \le F \le 0.211$.

Conclusions

An algorithm has been proposed to compute bounds on the flexibility index of processes described by nonlinear algebraic or dynamic models. It relies on the construction of two approximations to the feasibility test which can be used to determine the feasibility or infeasibility of regions within the uncertainty space. This can be used in a branch-and-bound algorithm to determine approximations to the feasible region and hence bounds on the flexibility index. The approach has been applied to three case studies and has been shown to identify the boundary of infeasible regions.

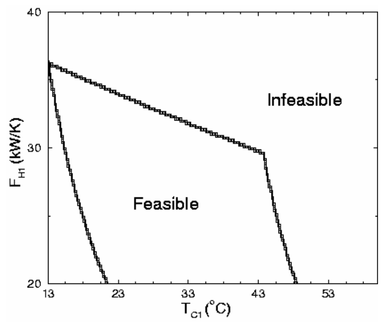

Fig. 3 – Feasible region for case study 3.

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