Korean J. of Chem. Eng., **6**(3) (1989) *200-205*

STABILITY OF A CFSTR WITH TWO CONSECUTIVE REACTIONS BY THE LIAPUNOV DIRECT METHOD

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(Received 22 August 1988 • accepted 27 January 1989)

Abstract—The stability of a continuous flow stirred tank reactor with two consecutive reactions $A \rightarrow B \rightarrow C$ is studied with the direct method of Liapunov. Krasovskii's method with the identity matrix is used to obtain a Liapunov function in the analysis of the system with single or multiple steady states. The results show that this method is mathematically conservative as expected. From the viewpoint of practical stability, however, this method predicts the regions of stability adequately.

INTRODUCTION

In the previous paper[1], we have investigated the sensitivity and the parametric sensitivity of a CFSTR with two consecutive reactions. In this study, we consider the stability of the reactor system by the direct method of Liapunov. The goal of this analysis is to examine the local stability of a steady state and determine the regions of stability.

The region of stability about a steady state is defined as the set of initial conditions from which the system trajectories will return to the steady state. When multiple steady states exist, there should be separatrices which divide the whole phase space into the region of stability for each steady state. The location of these separatrices for a single reaction system can be determined by the direct integration of the governing equations. But for the consecutive reactions system, extensive calculation is necessary to locate separatrices in the three-dimensional phase space. Therefore, Liapunov direct method has a greater potential for treating this three-dimensional problem.

In the present paper, we apply the direct method of Liapunov for a unique steady state system considered in the previous paper. Although the method was found too conservative mathematically, this method can give meaningful results from the viewpoint of practical stability.

LIAPUNOV DIRECT METHOD

In order to analyze the stability by the Liapunov second method, let us first consider a dynamic system which satisfies the equation

$$\frac{d\mathbf{x}_a(t)}{dt} = \mathbf{F}[\mathbf{x}_a(t)] \tag{1}$$

where $\mathbf{F}$ may be linear or nonlinear in $\mathbf{x}_a$. We shall assume that this system has a steady state $\mathbf{c}$. Then

$$\mathbf{F}(\mathbf{c}) = \mathbf{0}.$$

To investigate the stability we transform the coordinates as $\mathbf{x} = \mathbf{x}_a - \mathbf{c}$ and write the equation in $\mathbf{x}$ a follows:

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}), \quad \mathbf{f}(\mathbf{0}) = \mathbf{0}. \tag{2}$$

Now we consider two regions, $|\mathbf{x}| \leq \delta$ and $|\mathbf{x}| < \epsilon$, inside a hypersphere R such that

$$\delta < \epsilon < R.$$

The stability of the system at a steady state $\mathbf{x} = \mathbf{0}$ is defined as follows:

[Definition 1] A steady state is stable if for every radius ϵ there exists a radius δ such that if a trajectory starts at a point $\mathbf{x}_0$ inside the region of radius δ (or on that hypersphere), then if will always remain in the hyperspherical region of radius ϵ (or on that hypersphere).

[Definition 2] A steady state is asymptotically stable if it is stable and if every trajectory starting inside some hyperspherical region in the state space converges to the origin as the time tends to infinity.

We also need definitions on the positive definiteness and the Liapunov function.

[Definition 3] A scalar function $V(\mathbf{x})$ is positive definite when

i) $V(\mathbf{0}) = 0$,

ii) $V(\mathbf{x}) > 0$ for $\mathbf{x} \in S$, where $\mathbf{x} \neq \mathbf{0}$ and S refers to the state space,

iii) $V(\mathbf{x})$ is continuous in S, and

iv) $\partial V(\mathbf{x})/\partial x_i$, $i = 1, \cdots n$ are also continuous.

If the inequality sign is reversed, $V(\mathbf{x})$ is said to be negative definite.

[Definition 4] A scalar function $V(\mathbf{x})$ is said to be a Liapunov function when

i) $V(\mathbf{x})$ is positive definite, and

ii) $dV(\mathbf{x})/dt$ along a trajectory is negative definite or negative semi-definite (i.e., ≤ 0).

Then the stability and asymptotic stability theorems are given as follows:

[Theorem 1] *Stability theorem*: If there exists a Liapunov function $V(\mathbf{x})$ in some region S around a steady state, then the steady state is stable for all $\mathbf{x}_0$ contained in S.

[Theorem 2] *Instability theorem*: If $V(\mathbf{x})$ is continuous and if $dV(\mathbf{x})/dt$ along a trajectory is negative definite, then the system is unstable in that finite region of the state space for which $V(\mathbf{x})$ is not positive semi-definite.

The proof of these theorems will not be given here. If the stability theorems are satisfied everywhere in the state space, then the limitations to a region S imposed in the theorems may be deleted. The steady state $\mathbf{0}$ is then globally stable.

From the above theorems, in principle, we can determine the stability of a steady state and the region of the stability around the steady state. Quite often, however, it is very difficult to find a Liapunov function in the state space. The Liapunov direct method provides only the sufficient condition for the stability. Therefore the method gives inconclusive results when it is failed to find a Liapunov function. Therefore, the method should be applied with this in mind.

KRASOVSKII'S METHOD

Several methods have been suggested for obtaining the Liapunov function $V(\mathbf{x})$. In this analysis of complex reaction systems, we decided to use Krasovskii's method since this was successfully applied to single reaction systems by Perlmutter [2]. Kasovskii's Liapunov function has the following quadratic form in the $\mathbf{f}$ space:

$$V(\mathbf{x}) = \mathbf{f}^T \mathbf{P} \mathbf{f} \tag{3}$$

where the symmetric matrix $\mathbf{P}$ should be positive definite in order that $V(\mathbf{x})$ is positive definite.

The time derivative of $V(\mathbf{x})$ along a trajectory is

$$\dot{V}(\mathbf{x}) = \frac{dV}{dt} = \frac{\partial \mathbf{f}^T}{\partial t} \mathbf{P} \mathbf{f} + \mathbf{f}^T \mathbf{P} \frac{\partial f}{\partial t} \tag{4}$$

Noting that

$$\frac{\partial \mathbf{f}}{\partial t} = \frac{\partial \mathbf{f}}{\partial \mathbf{x}} \frac{d\mathbf{x}}{dt} = \mathbf{J} \mathbf{f} \tag{5a}$$

and

$$\frac{\partial \mathbf{f}^T}{\partial t} = (\mathbf{J}\mathbf{f})^T = \mathbf{f}^T \mathbf{J}^T, \tag{5b}$$

we rewrite Eqn (5) in the following form:

$$\dot{V}(\mathbf{x}) = -\mathbf{f}^T \mathbf{Q} \mathbf{f} \tag{6}$$

where $\mathbf{Q} = -(\mathbf{P}\mathbf{J} + \mathbf{J}^T\mathbf{P})$ and $\mathbf{J}$ represents the Jacobian matrix $\partial \mathbf{f}/\partial \mathbf{x}$. Then, if $\mathbf{Q}$ is positive definite [$\dot{V}(\mathbf{x})$ is negative definite] in some region, $V(\mathbf{x})$ is a Liapunov function and the steady state is stable in the region. In this analysis, we first choose a positive definite matrix $\mathbf{P}$ and then determine the region where $\dot{V}(\mathbf{x})$ is negative definite.

For the stability analysis of the consecutive reaction system by the Liapunov direct method, we write the governing equations given in the previous paper in dimensionless form:

$$\frac{dx}{d\tau} = 1 - \left(1 + Da_1 \exp\left[\gamma_1 \frac{z-1}{z}\right]\right) x = f_1 \tag{7}$$

$$\frac{dy}{d\tau} = Da_1 \exp\left[\gamma_1 \frac{z-1}{z}\right] x - \left(1 + Da_2 \exp\left[\gamma_2 \frac{z-1}{z}\right]\right) y = f_2 \tag{8}$$

$$\frac{dz}{d\tau} = (1 + \kappa_w) - (1 + \kappa) z + \beta_1 Da_1 \exp\left[\gamma_1 \frac{z-1}{z}\right] x + \beta_2 Da_2 \exp\left[\gamma_2 \frac{z-1}{z}\right] y = f_3 \tag{9}$$

where the symbols are explained in the Nomenclature.

In this study, $V(\mathbf{x})$ is determined in the $\mathbf{x}$ space (concentration-temperature space) by a geometrical method as follows. For a given T, V is given by a second order polynomial with respect to C_A and C_B in the isothermal plane since $\mathbf{f}$ is a linear function in C_A or C_B. In other words, contours of constant V will have forms of conic sections in a given isothermal plane. $\dot{V}(\mathbf{x})$ is given by a third order polynomial since each element of $\mathbf{J}$ is also linear with respect to C_A or C_B. In determining the region where $\dot{V}(\mathbf{x})$ is negative definite, the boundary where $\dot{V}(\mathbf{x}) = 0$ at a given isothermal plane is determined first by the Cardan's method, and then the region is selected by examining the sign of $\dot{V}(\mathbf{x})$ at $C_A = C_B = 0$. The maximum $V(\mathbf{x})$ keeping $\dot{V}(\mathbf{x})$ negative definite is determined first at each isothermal plane, and then the least upper bound (lub) of $V(\mathbf{x})$ is determined in the state space of C_A, C_B and T.

For the positive definite matrix $\mathbf{P}$ we choose the identity matrix $\mathbf{I}$ since $\mathbf{I}$ is the simplest positive definite matrix and requires the minimum level of calculation. In Fig. 1, some of the contours of $V(\mathbf{x})$ and the regions where $\dot{V}(\mathbf{x})$ are positive difinite are shown at some constant z planes when only one steady state exists. The numerical values of the parameters are given in Table 1. It

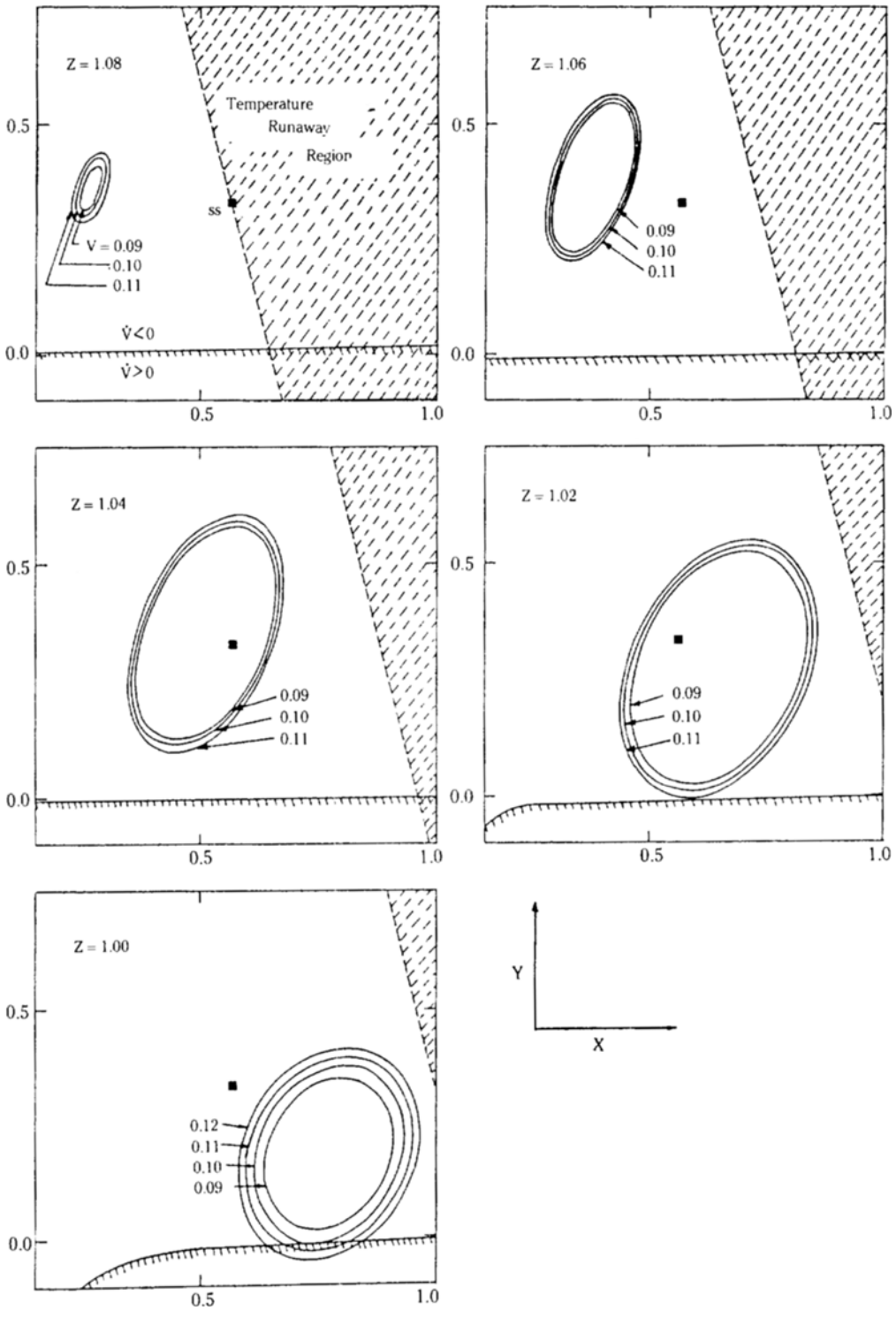

Fig. 1. Determination of the region of stability by the geometrical method.

Table 1. Numerical values of the system and operating parameters for a unique steady state system

Da_1	:	0.27114	Da_2	:	0.11795
γ_1	:	33.303	γ_2	:	34.735
β_1	:	0.42941	β_2	:	0.21471
κ	:	10.0	z_w	:	1.01471

should be noted in Fig. 1 that the region where $\dot{V}>0$ shrinks as z takes a smaller value. Especially, when $z<1.06$, the region is below $y=0$, outside of the physical values. When the dimensionless temperature z is equal to 1, the ellipse $V(\mathbf{x})=0.1$ is tangent to the locus $\dot{V}(\mathbf{x})=0$. When $z>1.02$, the ellipse $V(\mathbf{x})=0.1$ remains in the region where $\dot{V}(\mathbf{x})$ is negative definite. The size of the cross-section of the three dimensional surface $V=0.1$ takes the largest value when $z=1.02$ (See Fig. 2 for the ellipses at several different z values). Below this value the size shrinks rapidly and vanishes when $z=0.99$. Since the size of the cross section of $V=0.1$ takes a smaller value as z approaches 0.99 while keeping x and $y>0$, and the region where $\dot{V}$ is positive definite retreats below $y=0$ as stated earlier, $\dot{V}<0$ is confirmed in the region $V(x)=0$. Therefore, $\text{lub}\{\dot{V}(\mathbf{x})\}_{\dot{V}\le 0}=0.1$ for all values of z and the steady state is stable in the region where $V(\mathbf{x})<0.1$.

The region of stability so determined is very conservative mathematically for the system with a unique steady state. In other words, even when the steady state is stable in the whole region of (C_A, C_B, T) space, the region determined by Krasovskii's method with the identity matrix would be too small. Hence this method appears to have very limited applicability. As indicated above, this method gives only the sufficient condition for the stability. Moreover, it may be too conservative when found. However, we can give different interpretation from the viewpoint of practical stability. As shown in the previous paper, trajectories may deviate from the proper design criteria even when the steady state is unique. In this sense, guaranteeing the uniqueness may not be sufficiently safe in designing a reactor even when the steady state is asymtotically stable in the whole region. Conversely, when the system variables remain within the limits of design criteria, we can operate the reactor at a locally unstable steady state. Since there should exist small variations even in the case of so called steady operations, for example, a limit cycle with a small amplitude may be acceptable. Therefore we need a stability concept in practical sense. La Salle and Lefschetz [3] introduced the concept of practical stability for this purpose. In the following, we apply the concept of practical stability for the analysis of the consecutive reactions system.

In the previous paper, we showed the existence of parametric sensitivity depending upon the system and operating parameters for a given set of the initial conditions. In Fig. 1, the regions of initial conditions which lead to temperature runaway are shown at some isothermal planes. In the figure we note that the temperature runaway regions expand as the initial temperature takes higher values. The locus $V(\mathbf{x})=0.1$

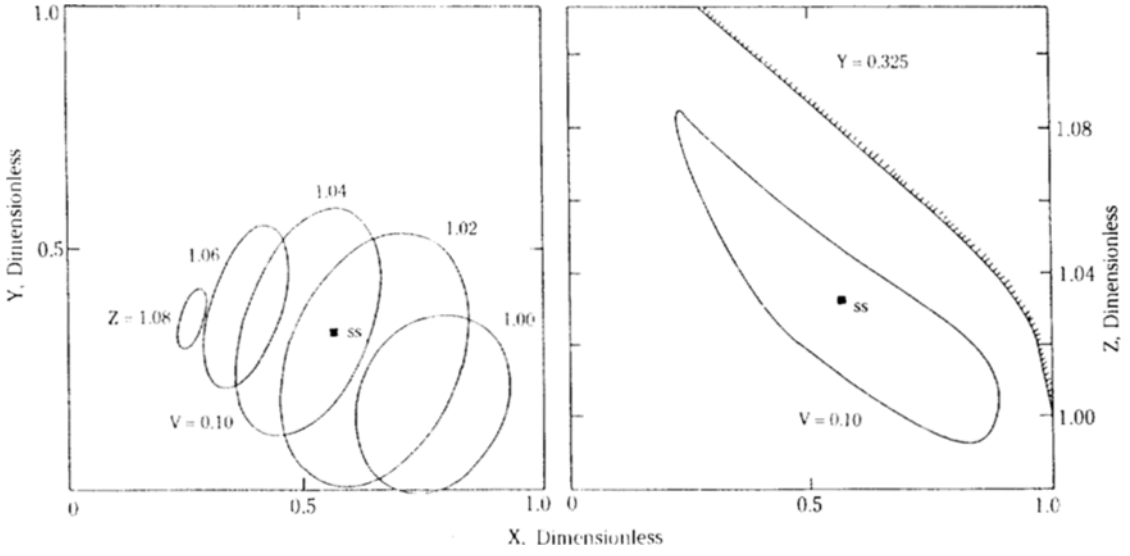

Fig. 2. Region of asymptotic stability: Projections of $V=0.1$ on the $z=$ const. planes and on the $y=$ const. plane. The upper right corner of the $y=0.325$ plane represents the temperature runaway region. ss: steady state.

Table 2. Numerical values of the system and operating parameters for a five steady states system

Da_1	:	0.03738	Da_2	:	4.3487×10^{-8}
γ_1	:	53.433	γ_2	:	81.412
β_1	:	0.22668	β_2	:	0.19430
$\varkappa$	:	0.2	z_w	:	0.96503

also moves toward that direction and does not intersect the temperature runaway region. Therefore we can conclude that the Liapunov function obtained by Krasovskii's method with the identity matrix appropriately predicts the region of practical stability especially at high concentrations of C_A and C_B. At low concentrations, the Liapunov function is not practically important as it is not necessary to consider the region of negative concentrations. Therfore, the region of stability determined by this method may not be regarded too conservative.

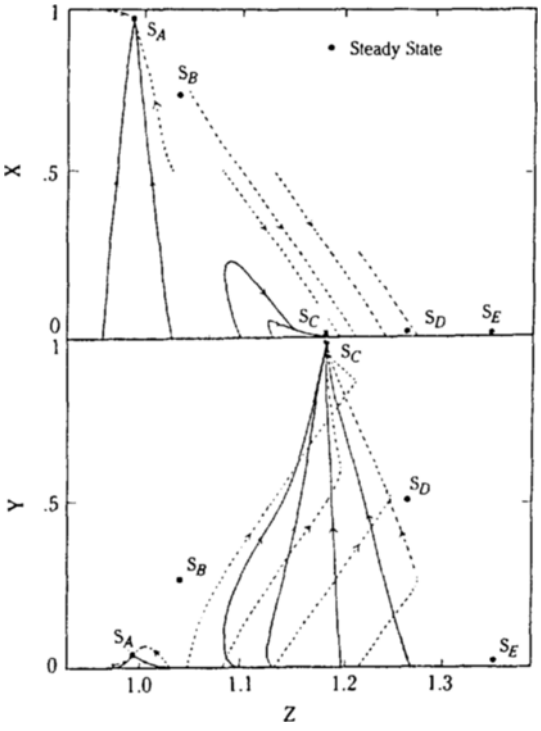

Fig. 3. Phase space plot for the five steady states system. Three dimensional trajectories are projected onto the coordinate planes. To distinguish the different set of initial conditions with the same initial temperature, dotted and solid lines are used. The numerical values of the parameters are given in Table 2.

Next we apply this method to a system with five steady states. The numerical values of the system and operating parameters are shown in Table 2. To test the validity of the Krasovskii's method with the identity matrix, we first integrate the governing equations by the Runge-Kutta fourth order scheme to obtain several trajectories as shown in Fig. 3. However, we could not locate the separatrices even after extensive calculation. Also, the trajectories which converge to the steady state S_E (the highest temperature case) could not be obtained easily because of the phenomenon of parametric sensitivity. With the Krasovskii's method, the region of stability around the highest temperature steady state could not be obtained, either. This implies that Krasovskii's method with the identity matrix could be useful in the estimation of the region of practical stability.

SUMMARY

In the present study, the stability of a CFSTR with two consecutive reactions has been analyzed by the Liapunov direct method. In obtaining a Liapunov function, we have used Krasovskii's method with the identity matrix. We tested this method for single and multiple steady states systems. In the former, asymptotic stability is guaranteed in the whole phase space so that the conservativeness of the method can be tested easily.

The result shows that the method is mathematically too conservative as expected. From the viewpoint of practical stability, however, this method appears to predict the region of stability adequately. For robustness of this conclusion, more examples should be tested.

NOMENCLATURE

- $\mathbf{c}$: equilibrium state of $\mathbf{x}_a$
- Da : Damköler number
- $\mathbf{F}$: vector function [see Eqn (1)]
- $\mathbf{f}$: vector function [see Eqn (2)]
- $\mathbf{I}$: identity matrix
- $\mathbf{J}$: Jacobian matrix
- n : number of state variables
- $\mathbf{P}$: positive definite matrix
- $\mathbf{Q} = -(\mathbf{PJ} + \mathbf{J}^T\mathbf{P})$
- R : radius of the hypersphere
- S : region around a steady state
- t : time
- V : scalar function or Liapunov function
- $\mathbf{x}_a$: state variable
- $\mathbf{x}$: $\mathbf{x}_a$-$\mathbf{c}$

x : dimensionless concentration of A (scale: feed conc. of A)
y : dimensionless concentration of B (scale: feed conc. of A)
z : dimensionless reactor temperature (scale: feed temperature)

Greek Letters

β : parameter representing the heat of reaction
γ : parameter representing the activation energy
δ : small parameter
ε : small parameter
$\varkappa$: parameter representing the heat transfer coefficient
τ : dimensionless time (scale: mean residence time)

Subscripts

f : feed
w : wall
1 : reaction $A \rightarrow B$
2 : reaction $B \rightarrow C$

Superscript

T : transpose

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