

DETERMINATION OF HOPF BIFURCATION SETS OF A CHEMICAL REACTORS BY TWO-PARAMETER CONTINUATION METHOD

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A two-parameter continuation method was developed and shown in the form of an example, allowing determination of Hopf bifurcation sets in a chemical reactor model. Exemplary calculations were made for the continuous stirred tank reactor model (CSTR). The set of HB points limiting the range of oscillation in the reactor was determined. The results were confirmed on the bifurcation diagram of steady states and on time charts. The method is universal and can be used for various models of chemical reactors.

Keywords: chemical reactor, Hopf bifurcation, tank reactor, bifurcation diagram, steady states, stability, dynamics

1. INTRODUCTION

The graphic presentation of equation solutions of the reactor model are the so-called steady state diagrams. Some of these states are stable, while others may be unstable. One type of instability is the loss of stationarity in favour of oscillation. This phenomenon was called in the scientific literature Hopf bifurcation (HB), and the transition point from stationary state to oscillations was called the Hopf bifurcation point.

This article has developed a method that allows to determine the set of HB points limiting the areas of oscillation. The method is based on a two-parameter continuation algorithm (Berezowski, 2010). It is easy to use and can be inserted into a computer program as a subprogram and does not require the use of large IT systems.

In this work, this method was used to determine the set of HB points for the CSTR model. There are many studies in the scientific literature on the model of a tank reactor (Agrawal et al., 1982; Antonelli et al., 2003; Berezowski et al., 2009; Berezowski, 2017; Chen et al., 1996; Kubíček et al., 1980; Merta, 2006; Starzak et al., 1990; Verazaluce-García, 2000; Żukowski et al., 2000). So far, however, no such algorithm has been developed or presented.

This method should therefore be applied at the reactor system design stage. It can also be used for basic scientific research. One of the main features of this method is tracking the HB line by observing the determinant of the appropriate Jacobi matrix, which greatly simplifies the calculation. The method is universal and can be used for many mathematical models of chemical reactors.

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2. REACTOR MODEL AND CALCULATION ALGORITHM

It was assumed that a single n -order $A \rightarrow B$ type reaction takes place in CSTR. Therefore, the balance equations are as follows:

- mass balance:

$$\frac{\partial \alpha}{\partial \tau} = -\alpha + \phi(\alpha, \theta) = f_1 \quad (1)$$

- heat balance:

$$\frac{d\theta}{d\tau} = \frac{1}{Le} [-\theta + \phi(\alpha, \theta) + \delta(\theta_H - \theta)] = f_2 \quad (2)$$

where ϕ is a function of kinetics reaction in the form:

$$\phi = D_a (1 - \alpha)^n \exp\left(\gamma \frac{\beta\theta}{1 + \beta\theta}\right) \quad (3)$$

To determine Hopf bifurcation points, the first Lyapunov's method based on linearization of the model (1)–(3) around the steady state was used. As a result, the matrix system was obtained:

$$\frac{d\bar{x}}{d\tau} = \bar{A}\bar{x} \quad (4)$$

where:

$$\bar{x} = \begin{bmatrix} \alpha - \alpha_s \\ \theta - \theta_s \end{bmatrix} \quad (5)$$

$$\bar{A} = \begin{bmatrix} \frac{\partial f_1}{\partial \alpha_s} & \frac{\partial f_1}{\partial \theta_s} \\ \frac{\partial f_2}{\partial \alpha_s} & \frac{\partial f_2}{\partial \theta_s} \end{bmatrix} \quad (6)$$

The characteristic equation of the linear state, Eq. (4), is:

$$\det(\bar{A} - \lambda \bar{E}) = 0 \quad (7)$$

According to the Hopf bifurcation definition, this is the point where the real part of the complex eigenvalue λ is equal to zero. This part is expressed as:

$$Re(\lambda) = \frac{1}{2} \left(\frac{\partial f_1}{\partial \alpha_s} + \frac{\partial f_2}{\partial \theta_s} \right) = f_3 \quad (8)$$

Hopf bifurcation is therefore determined by the following system of 3 equations:

$$f_1(\alpha_s, \theta_s, c, p) = 0 \quad (9)$$

$$f_2(\alpha_s, \theta_s, c, p) = 0 \quad (10)$$

$$f_3(\alpha_s, \theta_s, c, p) = 0 \quad (11)$$

where c and p are any chosen parameters of the reactor model.

The set of HB points can be determined from Eqs. (9)–(11) using the following two-parameter continuation procedure:

$$\begin{bmatrix} \alpha_{s,k+1} \\ \theta_{s,k+1} \\ c_{k+1} \end{bmatrix} = \begin{bmatrix} \alpha_{s,k} \\ \theta_{s,k} \\ c_k \end{bmatrix} - \bar{J}_k^{-1} \bar{w}_k \Delta p \operatorname{sign} \left[\det(\bar{J}_k) \right] \quad (12)$$

$$p_{k+1} = p_k + \Delta p \operatorname{sign} \left[\det \left(\bar{J}_k \right) \right] \quad (13)$$

where $\operatorname{sign} \left[\det \left(\bar{J}_k \right) \right]$ is the sign of the determinant of Jacobi \bar{J}_k , i.e. a number equal to 1 or -1 . It allows us to track the direction of movement of the HB point on the plot. The index k is the next point number on the chart.

The Jacobi \bar{J} matrix and the vector \bar{w} are as follows:

$$\bar{J} = \begin{bmatrix} \frac{\partial f_1}{\partial \alpha_s} & \frac{\partial f_1}{\partial \theta_s} & \frac{\partial f_1}{\partial c} \\ \frac{\partial f_2}{\partial \alpha_s} & \frac{\partial f_2}{\partial \theta_s} & \frac{\partial f_2}{\partial c} \\ \frac{\partial f_3}{\partial \alpha_s} & \frac{\partial f_3}{\partial \theta_s} & \frac{\partial f_3}{\partial c} \end{bmatrix} \quad (14)$$

$$\bar{w} = \begin{bmatrix} \frac{\partial f_1}{\partial p} \\ \frac{\partial f_2}{\partial p} \\ \frac{\partial f_3}{\partial p} \end{bmatrix} \quad (15)$$

where:

$$\frac{\partial f_3}{\partial \alpha_s} = \frac{\partial^2 f_1}{\partial \alpha_s^2} + \frac{\partial^2 f_2}{\partial \alpha_s \partial \theta_s} \quad (16)$$

$$\frac{\partial f_3}{\partial \theta_s} = \frac{\partial^2 f_1}{\partial \alpha_s \partial \theta_s} + \frac{\partial^2 f_2}{\partial \theta_s^2} \quad (17)$$

3. CALCULATIONS AND ANALYSIS OF THE RESULTS

The following values of the reactor parameters were taken for calculations: $\gamma = 15$, $\beta = 2$, $\delta = 3$, $n = 1.5$, $Le = 1$. Assuming $c = \theta_H$, $p = Da$, a set of HB points was determined as in Fig. 1.

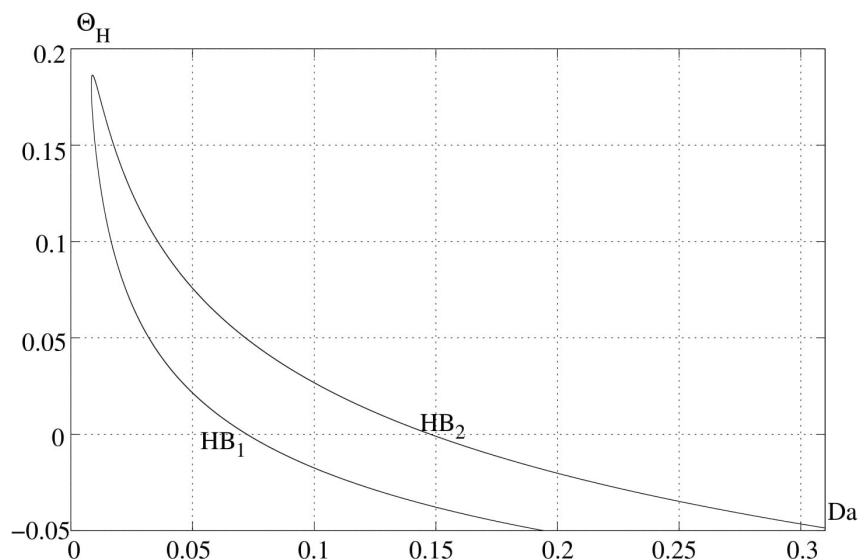


Fig. 1. Hopf bifurcations set

Assuming $\theta_H = 0$ in Fig. 2 the bifurcation diagram is shown, and the location of two Hopf bifurcation points HB_1 and HB_2 is marked on it.

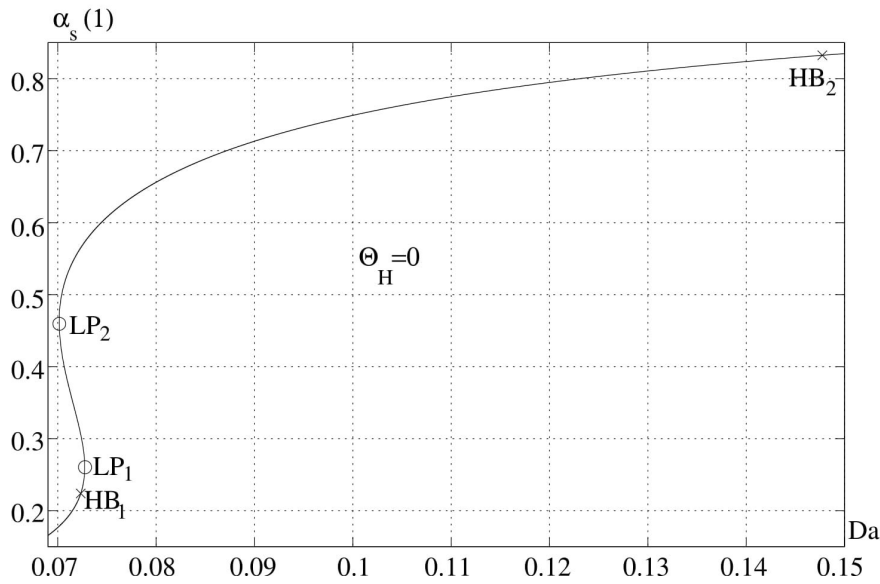


Fig. 2. Bifurcation diagram

It can be seen that they exactly correspond to HB points in Fig. 1. Because the diagram shown is characterized by the multiple of steady-state states, it also has 2 characteristic boundary points, namely LP_1 and LP_2 .

To confirm the results obtained, the following figures depict time series for $\theta_H = 0$ and for three different Da values, concerning three different places on the chart in Fig. 1. Thus, Fig. 3 presents the time series of the variable α for $Da = 0.05$.

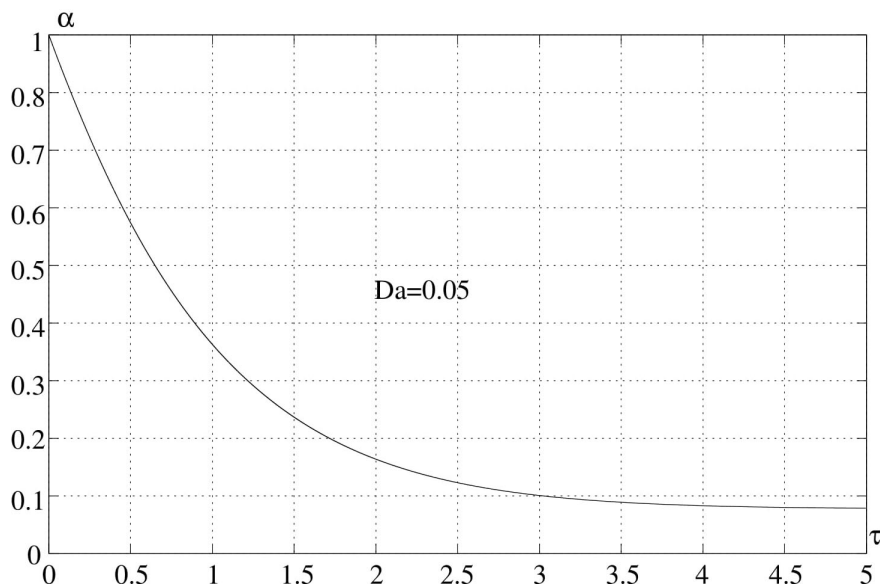


Fig. 3. Time series. Lower stable steady-state outside area of Hopf bifurcations

It corresponds to a point outside HB area. It is clear that we are dealing here with a stable steady state. Figure 4 shows the time series of the variable α for $Da = 0.1$.

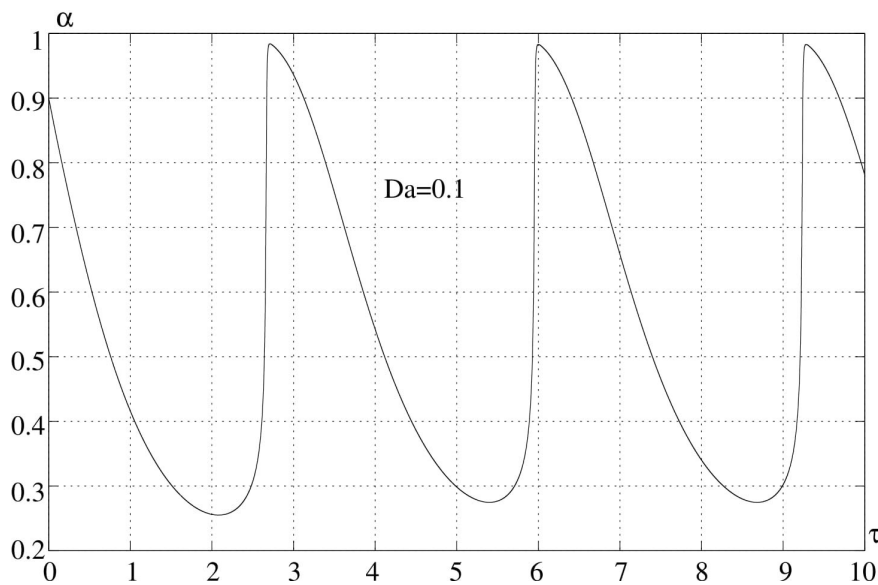


Fig. 4. Time series. Oscillations inside area of Hopf bifurcations

It corresponds to a point located inside the HB area. It is clear that we are dealing with oscillations. Fig. 5 shows the time series of the variable α for $Da = 0.2$.

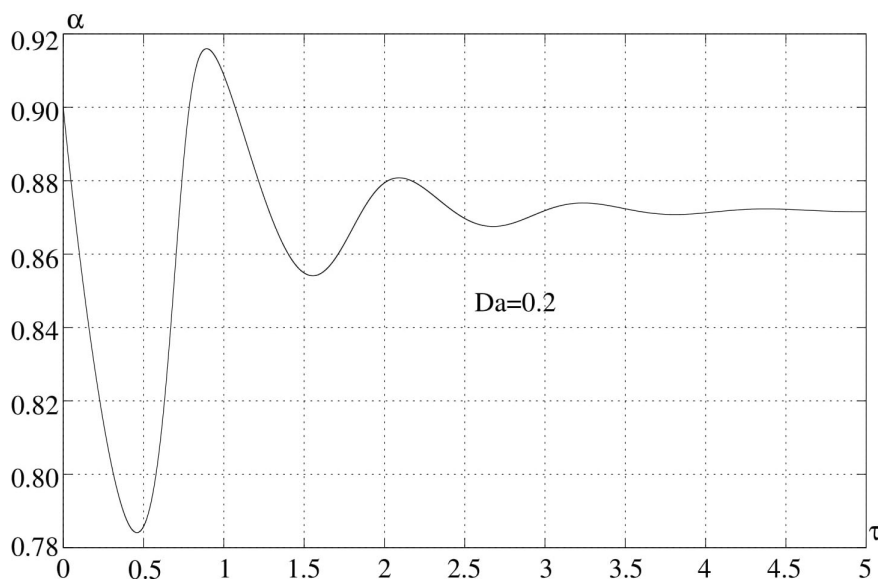


Fig. 5. Time series. Upper stable steady-state outside area of Hopf bifurcations

It corresponds to a point outside HB area. It is clear that we are dealing here with a stable steady state. The above results have also been confirmed in the diagram in Fig. 2.

4. CONCLUSIONS

In this paper, a two-parameter continuation method was developed to determine the areas of Hopf bifurcation of a chemical reactor. Exemplary calculations were made using the tank reactor model. The set of HB points determining the occurrence of oscillations was determined. The results were confirmed on the

bifurcation diagram of steady states and on the time series plots. The method presented in this paper is a universal one and is applicable for various types of chemical reactor models.

SYMBOLS

c_p	heat capacity, kJ/(kg K)
C_A	concentration of component A, kmol/m ³
Da	Damköhler number $\left(= \frac{V_R (-r_0)}{\dot{F} C_0}\right)$
E	activation energy, kJ/kmol
\dot{F}	volumetric flow rate, m ³ /s
$(-\Delta H)$	heat of reaction, kJ/kmol
k	reaction rate constant, 1/[s (m ³ /kmol) ^{$n-1$}]
Le	Lewis number
n	order of reaction
$(-r)$	rate of reaction, (= kC^n), kmol/(m ³ s)
R	gas constant, kJ/(kmol K)
t	time, s
T	temperature, K
V	volume, m ³

Greek symbols

α	degree of conversion $\left(= \frac{C_{A0} - C_A}{C_{A0}}\right)$
β	dimensionless number related to adiabatic temperature increase $\left(= \frac{(-\Delta H) C_{A0}}{T_0 \rho c_p}\right)$
γ	dimensionless number related to activation energy $\left(= \frac{E}{RT_0}\right)$
δ	dimensionless heat exchange coefficient $\left(= \frac{A_q k_q}{\rho c_p \dot{F}}\right)$
λ	eigenvalue
θ	dimensionless temperature $\left(= \frac{T - T_0}{\beta T_0}\right)$
ρ	density, kg/m ³
τ	dimensionless time $\left(= \frac{\dot{F}}{V_R} t\right)$

Subscripts

0	refers to feed
H	refers to temperature of cooling medium
R	refers to reactor
s	stationary state

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