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Chaotic oscillations of coupled chemical reactors

Marek Berezowski [a,*], Daniel Dubaj [b]

[a] Silesian University of Technology, Faculty of Applied Mathematics, 44–100 Gliwice, ul. Kaszubska 23, Poland

[b] Cracow University of Technology, Faculty of Chemical Engineering and Technology, 31–155 Kraków, ul. Warszawska 24, Poland

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ABSTRACT

The scope of the paper is the dynamics of chemical reactors with double recycle, which may generate complicated oscillations, including chaotic ones. Such system does not only have multiple steady states, but also multiple dynamic states, which was demonstrated on the examples of steady sixth periodic orbits.

1. Introduction

One of the methods of intensifying the operation of chemical reactors is the use of the mass-heat recycle loops. A part of non-reactionary flux is reintroduced to the system together with the feed. Generally, chemical reactors with mass and heat recycle have great significance and are widely used in industry. The use of recycle enables the recovery of the unreacted mass and enables the use of the heat of reaction to preheat the feed. Recycle also enables control of the system [1,2].

In practice, loops of relatively small volume are used. In the modeling of the loops it is assumed that they are adiabatic, have short residence time and do not enter into chemical reactions [3–5,7,8,10–14].

In this paper, however, the above principle was not followed, and, instead, a reactor was placed in the loop. Thus, a symmetrical system was created, consisting of two mutually coupled tubular reactors. The recycle flux from one of the reactors is introduced, together with the raw material flux to the second reactor, and, the other way round. Such system enables the achievement of higher degrees of conversion in comparison with a single reactor, and, in consequence, is more effective from the point of view of the process and economics.

In the system presented in this paper both multiple steady states, as well as multiple oscillations states can occur. If initial conditions of reactors are respectively different, then on the output of the whole system will occur states alternately connected with first or second reactor. This phenomenon has been shown in [6]. It is impossible to achieve this in the reactor with ordinary recycle.

2. Model of the system

The block diagram of the investigated system is shown in Fig. 1.

The raw material flux, with the contribution of 1, is fed to the system. Next, the flux is split into the input of the two reactors in accordance with division q. The volumetric contributions of the reactors are described by coefficient k_V. The output fluxes from the reactors are divided into the fluxes leaving the system and recycle fluxes. The degrees of such division are characterized by coefficients f_A and f_B. The flux from reactor A reaches the inlet of reactor B in quantity f_A, whereas, the flux from reactor B reaches the inlet of reactor A in quantity f_B. The remaining fluxes are mixed and leave the

* Corresponding author. Tel.: +48322372864; fax: +48322372864.
E-mail address: marek.berezowski@polsl.pl (M. Berezowski).

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Notations

Da	Damköhler number
f	recycle coefficient
k_V	dimensionless number related to volume of reactor
n	reaction order
q	dimensionless number related to division of substract stream
τ	dimensionless time
α	conversion degree
β	dimensionless number related to adiabatic temperature increase
δ	dimensionless heat exchange coefficient
γ	dimensionless number related to activation energy
Θ	dimensionless temperature
ζ	dimensionless position
σ	dimensionless residence time

Subscripts

A	refers to reactor A
B	refers to reactor B
H	refers to cooling medium

system in quantities$(1-f_A)$ and $(1-f_B)$, respectively. It was assumed that both reactors are homogeneous, without dispersion, and cooled by the agent with constant temperature Θ_H. To simplify the analysis, it was also assumed that in both reactors reactions $A\to B$ with the kinetics of the nth order occur, in accordance with Arrhenius equation described by function φ. Such assumption guarantees that the reaction as such does not generate dynamic phenomena (as Belousov–Zhabotinsky reaction, for example). Choice of a plug flow reactor model (without dispersion) excludes the possibility for the considered dynamical system to exhibit multiple steady states or periodic solution in absence of recycle.

The mathematical model of such system may be described by the following four partial differential equations:

$$\frac{\partial\alpha_A}{\partial\zeta_A}+\frac{\partial\alpha_A}{\partial\tau}=\varphi(\alpha_A,\Theta_A) \tag{1}$$

$$\frac{\partial\Theta_A}{\partial\zeta_A}+\frac{\partial\Theta_A}{\partial\tau}=\varphi(\alpha_A,\Theta_A)+\delta_A\cdot(\Theta_H-\Theta_A) \tag{2}$$

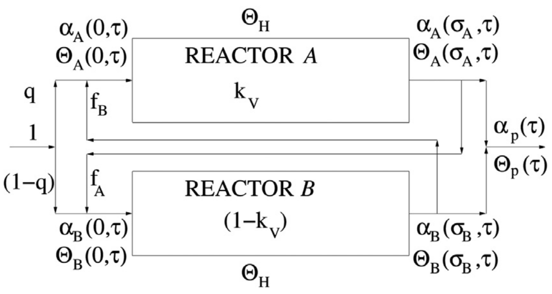

Fig. 1. Scheme of the system.

$$\frac{\partial\alpha_B}{\partial\zeta_B}+\frac{\partial\alpha_B}{\partial\tau}=\varphi(\alpha_B,\Theta_B) \tag{3}$$

$$\frac{\partial\Theta_B}{\partial\zeta_B}+\frac{\partial\Theta_B}{\partial\tau}=\varphi(\alpha_B,\Theta_B)+\delta_B\cdot(\Theta_H-\Theta_B). \tag{4}$$

The function of the kinetics of reaction $\varphi(\alpha_i,\Theta_i)$ has the form:

$$\varphi(\alpha_i,\Theta_i)=\mathrm{Da}(1-\alpha_i)^n\exp\left(\gamma\frac{\Theta_i\beta}{1+\Theta_i\beta}\right);\quad i=A,B. \tag{5}$$

The boundary conditions resulting from the mixing of the fluxes at the recycle points are:

$$\alpha_A(0,\tau)=f_B\cdot w\cdot\alpha_B(\sigma_B,\tau) \tag{6}$$

$$\Theta_A(0,\tau)=f_B\cdot w\cdot\Theta_B(\sigma_B,\tau) \tag{7}$$

$$\alpha_B(0,\tau)=f_A\cdot\frac{1}{w}\cdot\alpha_A(\sigma_A,\tau) \tag{8}$$

$$\Theta_B(0,\tau)=f_A\cdot\frac{1}{w}\cdot\Theta_1(\sigma_A,\tau) \tag{9}$$

where:

$$w=\frac{(1-q)+f_A\cdot q}{q+f_B(1-q)} \tag{10}$$

whereas, σ_A and σ_B are the coefficients that determine the residence time in the reactors:

$$\sigma_A=\frac{k_V}{w};\quad\sigma_B=k_Vw. \tag{11}$$

Upon solving the above equation, the values of the degrees of conversion and temperature at the outlet of the reactors are derived. The output flux from the entire system is an effect of the mixing of both fluxes that leave the reactors. The degree of the conversion and temperature in this flux is calculated from the following equations:

$$\alpha_P(\tau)=k_P\cdot\alpha_A(\tau)+(1-k_P)\alpha_B(\tau) \tag{12}$$

$$\Theta_P(\tau)=k_P\cdot\Theta_A(\tau)+(1-k_P)\Theta_B(\tau) \tag{13}$$

where:

$$k_P=\frac{q+f_2(1-q)}{1-f_1f_2}(1-f_1) \tag{14}$$

$$1-k_P=\frac{(1-q)+f_1q}{1-f_1f_2}(1-f_2). \tag{15}$$

According to scientific literature, a tubular reactor with a single recycle loop may generate various types of oscillations, from periodic to chaotic ones [1–8,10–14]. As far as the system investigated in this paper is concerned, it involves the mass-heat coupling of two reactors that work simultaneously. Such system is structurally symmetrical with two recycle loops. Hence, it could be supposed that the system may generate complicated oscillations, including chaotic ones. Due to the absence of dispersion in the reactors and the constant cooling temperature, changes in the concentrations and temperatures are rapid, as indicated in [11]. In the discussed case, the interval between the rapid changes may be shorter than the residence time. Therefore, the method