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Fractal structure of iterative time profiles of a tubular chemical reactor with recycle

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Abstract

The scope of the paper is the theoretical analysis of the time rate in which a chemical reactor reaches a stable stationary state or stable temperature and concentration oscillations of the fluid flux. The method used for the analysis is based on the so-called iterative time profiles, demonstrating a chaotic and fractal nature of some of the profiles. The results were presented in the form of two and three-dimensional graphs.

1. Introduction

The dynamics of a homogeneous tubular chemical reactor without dispersion and with external feedback was discussed, for example, in [1–5], where it was demonstrated that the concentration and temperature of the fluid flux may be constant in the steady state or may oscillate in the form of rectangular time wave. The oscillations may be more or less complex, depending on the periodicity of the time series of the above-mentioned variables of a given state. Due to an asymptotic nature of the changes occurring in the reactor, the time rate required for the system to reach a steady state is, from the theoretical point of view, infinitely long. In practice, however, it may be assumed that the reactor is in the steady state when the values of its variables are relatively close to the values of the theoretical state. Thus, the time rate required for the system to reach the steady state is limited and depends on the values of the reactor parameters as well as on the values of temperature and concentration of the fluid flux at the initial moment. The reactor subjected to the theoretical analysis is a homogeneous tubular chemical reactor without dispersion and with external mass recycle [1,3,5]. The time required for the reactor to reach the steady state was illustrated by means of various types of two and three-dimensional iterative time profiles [6]. The profiles were demonstrated to have a chaotic nature and fractal structure.

2. The model of the reactor and its iterative time profiles

The differential mass balance model of a chemical reactor with recycle [1,3] was analyzed in the following form:

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Notations

Da	Damköhler number
f	recycle coefficient
n	order of reaction
α	conversion degree
β	coefficient related to enthalpy of reaction
Θ	dimensionless temperature
δ	dimensionless heat transfer coefficient
γ	dimensionless activation energy
λ	eigenvalue
ξ	dimensionless position coordinate along reactor

Subscripts

0	initial condition
H	heat exchanger
s	fixed point

$$\frac{d\alpha_{k+1}(\xi)}{d\xi} = (1-f)\phi[\alpha_{k+1}(\xi), \Theta_{k+1}(\xi)] \tag{1}$$

$$\frac{d\Theta_{k+1}(\xi)}{d\xi} = (1-f)\{\phi[\alpha_{k+1}(\xi), \Theta_{k+1}(\xi)] + \delta[\Theta_H - \Theta_{k+1}(\xi)]\} \tag{2}$$

$$\alpha_{k+1}(0) = f\alpha_k(1); \quad \Theta_{k+1}(0) = f\Theta_k(1) \tag{3}$$

$$\phi(\alpha, \Theta) = Da(1-\alpha)^n \exp\left(\gamma \frac{\beta\Theta}{1+\beta\Theta}\right). \tag{4}$$

The purpose of the analysis was to determine the impact of the initial values of conversion degree $\alpha_0(1)$ and dimensionless temperature $\Theta_0(1)$ on the number of discrete time steps N required for the reactor to reach a stable steady state, that is stable stationary point or stable periodic orbit [6]. It was assumed that the steady state for the reactor is the state when the distance between the trajectory generated by the model (1)–(4) and the fixed point $\alpha_s(1)$, $\Theta_s(1)$ is not longer than the one determined by the following condition:

$$\left(\left|\frac{\alpha(1)-\alpha_s(1)}{\alpha_s(1)}\right| + \left|\frac{\Theta(1)-\Theta_s(1)}{\Theta_s(1)}\right|\right) * 100\% < \varepsilon. \tag{5}$$

The analysis was based on the catastrophic set shown in Fig. 1 [1,3], generated for the following values of the parameters: $Da = 0.15$, $n = 1.5$, $\gamma = 15$, $\beta = 2$, $\delta = 3$. Crossing of the lines SN, FB or HB of this set leads to the change in the multiplication factor (saddle-node bifurcation), generation of jump oscillations (flip bifurcation) or generation of quasi-periodic oscillations (Hopf bifurcation), respectively. Thus, right to the zone marked by the FB line, the temperature and concentration of the fluid flux are constant in the steady state, practically for any value of the recycle coefficient within the range of $0 < f < 1$. Accordingly, what we are dealing with are fixed stationary points. But, within the boundaries of the zone marked by the FB line, the temperature and concentration oscillate in the steady state in a jump way [3]. Accordingly, we are dealing with fixed points of oscillation solutions.

By analyzing the eigenvalues α of the model (1)–(5), it is possible to determine the "*power*" by means of which a given fixed point attracts trajectories. The most powerful attractor is the point for which all the eigenvalue modules are equal to zero, whereas the least powerful point is the one for which the module of at least one eigenvalue is equal to 1. The eigenvalues of k-periodic solution may be derived from the following relation:

$$\bar{y}_k = f^k \prod_{j=1}^{k} e^{\int_0^1 \bar{\bar{J}}_j d\xi} \bar{y}_0 = f^k \prod_{j=1}^{k} \bar{\bar{M}}_j \bar{y}_0 = f^k \bar{\bar{A}}_k \bar{y}_0 \tag{6}$$

where $\bar{\bar{J}}_j$ is Jacobi matrix of the right sides of Eqs. (1) and (2), whereas $\bar{y}$ is the state vector of the linear approximation of the equations. The monodromy matrix $\bar{\bar{M}}_j$ may be derived from the following equation: