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The implementation of a mathematical model of variously structured bioreactors cascades

Implementacja modelu matematycznego kaskad bioreaktorów o różnych strukturach

Abstract

This paper paper the results of the stationary characteristics of CSTR bioreactor cascades with a modifiable structure, obtained by the way of numerical experiments. As a technological example, the biodegradation of phenol was chosen.

Keywords: bioreactor, cascade, biodegradation, substrate inhibition

Streszczenie

W artykule przedstawiono charakterystykę stacjonarną kaskady bioreaktorów z idealnym wymieszaniem o modyfikowalnej strukturze, uzyskaną w wyniku eksperymentów numerycznych. Jako modelowy przypadek przyjęto biodegradację fenolu.

Słowa kluczowe: bioreaktor, kaskada, biodegradacja, inhibicja substratem

1. Introduction

Cascades of bioreactors are commonly applied in industry; for example, in biotechnology or wastewater treatment [1]. The model of the serial connection of bioreactors has already been obtained and well described [2]. A model of a cascade with an unlimited number of bioreactors may be attached in calculating a model of a tube plug-flow reactor [3]. A significant influence on cascade operation may also be the location of the inlet stream and the recirculation of the outlet stream. Productivity may be also increased by applying a cyclic reversed-flow [4]. For the mentioned case, chaotic solutions has been reported [5]. Work [6] proposes that if there is a cascade of two reactors which are operating under the same conditions, their composition of output streams are also the same.

The formulation and analysis of steady-state estimations are helpful in describing the operation regime. This work is inspired by the modified bioreactor cascades model, in which particular vessels can be connected in any way [7].

2. Experimental data

As a technological example, phenol biodegradation was chosen; the kinetics parameters are as follows: m_{max} = 0.569 h^{-1}; K = 0.018539 kgm^{-3}; K_i = 0.09937 kgm^{-3}; w_{BA} = 0.628 [8]. Fig. 1. presents the structure of the examined cascade with inlet and outlet streams.

The mathematical model may be defined by the mass balances of degraded substrate and biomass in each reactor. The balance of the degraded substrate is expressed by:

$$V_1 \frac{dc_{A1}}{dt} = F_{V1}c_{A0} - F_{V1}c_{A1} - V_1 \frac{1}{w_{BA}} \frac{\mu_{max} c_{A1} c_{B1}}{K + c_{A1} + \frac{c_{A1}^2}{K_i}} \tag{1}$$

$$V_2 \frac{dc_{A2}}{dt} = F_{V2}c_{A1} - F_{V2}c_{A2} - V_2 \frac{1}{w_{BA}} \frac{\mu_{max} c_{A2} c_{B2}}{K + c_{A2} + \frac{c_{A2}^2}{K_i}} \tag{2}$$

$$V_3 \frac{dc_{A3}}{dt} = F_{V3}c_{A1} - F_{V3}c_{A3} - V_3 \frac{1}{w_{BA}} \frac{\mu_{max} c_{A3} c_{B3}}{K + c_{A3} + \frac{c_{A3}^2}{K_i}} \tag{3}$$

where:

- V_i – volume of *i*th reactor;
- c_{Ai} – concentration of substrate in *i*th reactor;
- t – time;
- F_{Vi} – volumetric flow rate through *i*th reactor;
- K – saturation constant;
- c_{Bi} – concentration of biomass in *i*th reactor;

m_{max} – maximal rate of biomass growth;
K_i – inhibition constant;
w_{BA} – yield of biomass production.

Similarly, biomass balance in each bioreactor may be purposed:

$$V_1 \frac{dc_{B1}}{dt} = F_{V1} c_{B0} - F_{V1} c_{B1} - V_1 \frac{\mu_{max} c_{A1} c_{B1}}{K + c_{A1} + \frac{c_{A1}^2}{K_i}} \tag{4}$$

$$V_2 \frac{dc_{B2}}{dt} = F_{V2} c_{B1} - F_{V2} c_{B2} - V_2 \frac{\mu_{max} c_{A2} c_{B2}}{K + c_{A2} + \frac{c_{A2}^2}{K_i}} \tag{5}$$

$$V_3 \frac{dc_{B3}}{dt} = F_{V3} c_{B1} - F_{V3} c_{B3} - V_3 \frac{\mu_{max} c_{A3} c_{B3}}{K + c_{A3} + \frac{c_{A3}^2}{K_i}} \tag{6}$$

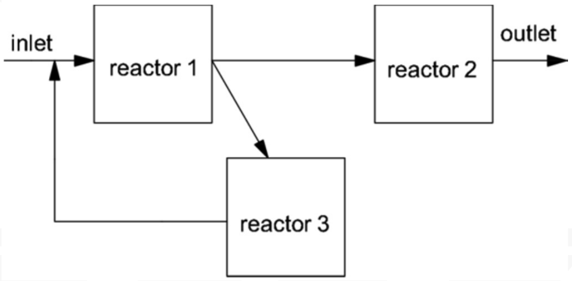

Fig. 1. Schematic drawing of investigated cascade

In the presented model, index *i* corresponds to the ordinal numbers of the reactors (as shown in Fig. 1). The concentration in the inlet stream is indicated by $i = 0$. In this work, it was assumed that all reactors have the same volume; thus:

$$V = V_1 = V_2 = V_3 \tag{7}$$

The total stream feeding the first reactor can be stated by the equation (8).

$$F_{V1} = F_{Vf} + F_{V3} \tag{8}$$

where:

F_{Vf} – volumetric flow rate of inlet stream.

Instead of no change to the total mass inside the cascade, it can be noted that volumetric flow rate of inlet and outlet stream are the same.

$$F_{Vf} = F_{V2} \tag{9}$$

Values c_{A0}, c_{B0} are expressed by the mass balance in the inlet of reactor 1:

$$F_{Vf}c_{Af} + F_{V3}c_{A3} = F_{V1}c_{A0} \tag{10}$$

$$F_{V3}c_{B3} = F_{V1}c_{B0} \tag{11}$$

Additionally, dimensionless variables will be introduced; degree of conversion the substrate in the *ith* bioreactor:

$$\alpha_{Ai} = \frac{c_{Af} - c_{Ai}}{c_{Af}} \tag{12}$$

dimensionless concentration of biomass in *i*th bioreactor:

$$\beta_i = \frac{c_{Bi}}{c_{Af}} \tag{13}$$

and average residence time in each bioreactor:

$$\tau_i = \frac{V}{F_{Vi}} \tag{14}$$

After substitution equations (7)–(11) to model (1)–(6), the dimensionless model of the investigated cascade is stated as:

$$\frac{d\alpha_{A1}}{dt} = \frac{\alpha_{A1}}{\tau_1} - \frac{\alpha_{A3}}{\tau_3} + \frac{1}{w_{BA}} \frac{\mu_{\max} c_{Af}(1-\alpha_{A1})\beta_1}{K + c_{Af}(1-\alpha_{A1}) + \frac{c_{Af}^2(1-\alpha_{A1})^2}{K_i}} \tag{15}$$

$$\frac{d\alpha_{A2}}{dt} = \frac{\alpha_{A2}}{\tau_2} - \frac{\alpha_{A1}}{\tau_2} + \frac{1}{w_{BA}} \frac{\mu_{\max} c_{Af}(1-\alpha_{A2})\beta_2}{K + c_{Af}(1-\alpha_{A2}) + \frac{c_{Af}^2(1-\alpha_{A2})^2}{K_i}} \tag{16}$$

$$\frac{d\alpha_{A3}}{dt} = \frac{\alpha_{A3}}{\tau_3} - \frac{\alpha_{A1}}{\tau_3} + \frac{1}{w_{BA}} \frac{\mu_{\max} c_{Af}(1-\alpha_{A3})\beta_3}{K + c_{Af}(1-\alpha_{A3}) + \frac{c_{Af}^2(1-\alpha_{A3})^2}{K_i}} \tag{17}$$

$$\frac{d\beta_1}{dt} = \frac{\beta_1}{\tau_1} - \frac{\beta_3}{\tau_3} + \frac{\mu_{\max} c_{Af}(1-\alpha_{A1})\beta_1}{K + c_{Af}(1-\alpha_{A1}) + \frac{c_{Af}^2(1-\alpha_{A1})^2}{K_i}} \tag{18}$$

$$\frac{d\beta_2}{dt} = \frac{\beta_2}{\tau_2} - \frac{\beta_1}{\tau_2} + \frac{\mu_{\max} c_{Af}(1-\alpha_{A2})\beta_2}{K + c_{Af}(1-\alpha_{A2}) + \frac{c_{Af}^2(1-\alpha_{A2})^2}{K_i}} \tag{19}$$

$$\frac{d\beta_3}{dt}=\frac{\beta_3}{\tau_3}-\frac{\beta_1}{\tau_3}+\frac{\mu_{\max} c_{Af}\left(1-\alpha_{A3}\right)\beta_3}{K+c_{Af}\left(1-\alpha_{A3}\right)+\frac{c_{Af}^2\left(1-\alpha_{A3}\right)^2}{K_i}} \tag{20}$$

Additionally, the average residence time in the cascade may be introduced as:

$$\tau=\frac{3V}{F_{Vf}} \tag{21}$$

From equations (9), (14) and (21), relations (22) can be obtained:

$$\tau=3\tau_2 \tag{22}$$

The division of stream F_{V1} may be characterised by parameter x:

$$x=\frac{F_{V3}}{F_{V2}} \tag{23}$$

Thanks to equations (8), (9), (22) and parameter x, the relations between residence times in each reactor and total residence time in the cascade could be obtained:

$$\tau_3=\frac{\tau}{3x} \tag{24}$$

$$\tau_1=\frac{\tau}{3(1+x)} \tag{25}$$

The final form of model in steady state is presented by equations (26)–(31):

$$0=\frac{3}{\tau}\left(x\alpha_{A3}-(1+x)\alpha_{A1}\right)+\frac{1}{w_{BA}}\frac{\mu_{\max} c_{Af}\left(1-\alpha_{A1}\right)\beta_1}{K+c_{Af}\left(1-\alpha_{A1}\right)+\frac{c_{Af}^2\left(1-\alpha_{A1}\right)^2}{K_i}} \tag{26}$$

$$0=\frac{3}{\tau}\left(\alpha_{A1}-\alpha_{A2}\right)+\frac{1}{w_{BA}}\frac{\mu_{\max} c_{Af}\left(1-\alpha_{A2}\right)\beta_2}{K+c_{Af}\left(1-\alpha_{A2}\right)+\frac{c_{Af}^2\left(1-\alpha_{A2}\right)^2}{K_i}} \tag{27}$$

$$\frac{3x}{\tau}\left(\alpha_{A1}-\alpha_{A3}\right)+\frac{1}{w_{BA}}\frac{\mu_{\max} c_{Af}\left(1-\alpha_{A3}\right)\beta_3}{K+c_{Af}\left(1-\alpha_{A3}\right)+\frac{c_{Af}^2\left(1-\alpha_{A3}\right)^2}{K_i}} \tag{28}$$

$$0=\frac{3}{\tau}\left(x\beta_3-(1+x)\beta_1\right)+\frac{\mu_{\max} c_{Af}\left(1-\alpha_{A1}\right)\beta_1}{K+c_{Af}\left(1-\alpha_{A1}\right)+\frac{c_{Af}^2\left(1-\alpha_{A1}\right)^2}{K_i}} \tag{29}$$

$$0=\frac{3}{\tau}(\beta_1-\beta_2)+\frac{\mu_{max}c_{Af}(1-\alpha_{A2})\beta_2}{K+c_{Af}(1-\alpha_{A2})+\frac{c_{Af}^2(1-\alpha_{A2})^2}{K_i}} \tag{30}$$

$$0=\frac{3x}{\tau}(\beta_1-\beta_3)+\frac{\mu_{max}c_{Af}(1-\alpha_{A3})\beta_3}{K+c_{Af}(1-\alpha_{A3})+\frac{c_{Af}^2(1-\alpha_{A3})^2}{K_i}} \tag{31}$$

It can be noted that the solution of the presented model may be continued by the three main process parameters: c_{Af}, x and τ. This has been achieved through the use of continuation and bifurcation tools. The continuation was realised for two concentrations of substrate in the feed: c_{Af} = 0.5 kgm^{-3} and c_{Af} = 1 kgm^{-3}. After the initial backward continuation for x = 0.4, forward two-parametric continuation was realised in order to obtain the catastrophic graphs. Continuation was then realised for three representative values of x: 0.4, 0.8 and 1.2.

3. Results

3.1. Catastrophic plots

Obtained plots are presented in Fig. 2a and Fig. 2b.

In both cases, the washout area (region I) lies in the same place. Regions of the fivefold steady state (III and V) are wider, when c_{Af} is higher. The other regions are triple steady states.

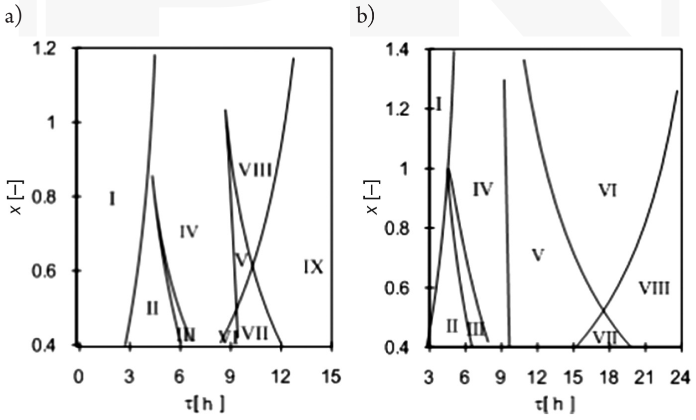

Fig. 2. Catastrophic plots of the investigated cascade (upper): a) for c_{Af} = 0.5 kgm^{-3} and (lower), b) for c_{Af} = 1 kgm^{-3}. Catastrophic sections are numbered by I–IX

3.2. Branches of steady states

Figs. 3 & 4 present branches of steady states for the three selected values of x parameter: $x = 0.4$, $x = 0.8$ and $x = 1.2$.

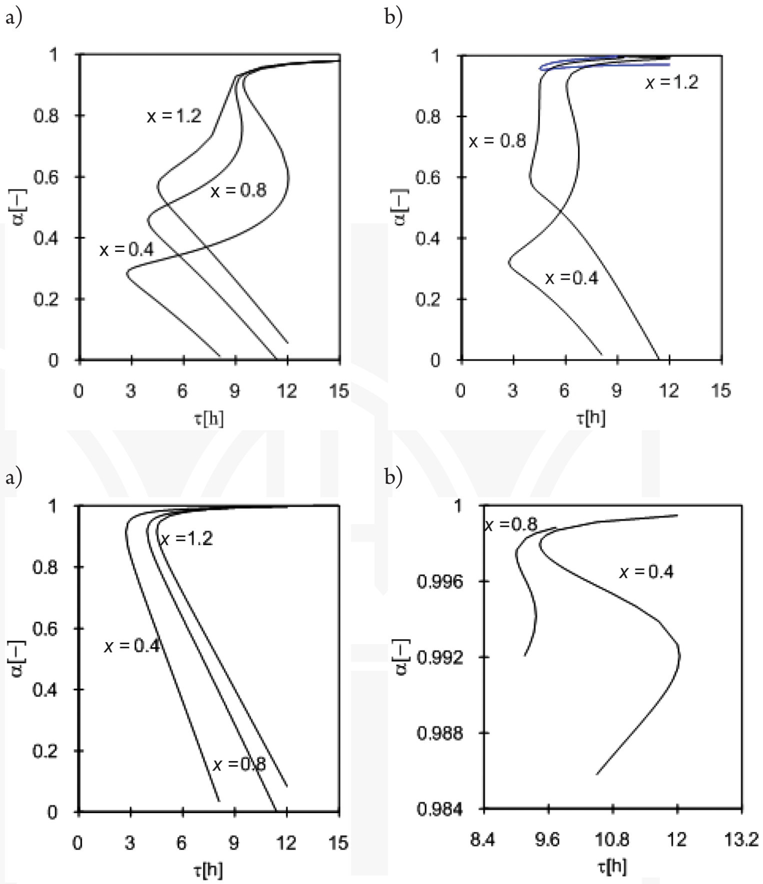

Fig. 3. Branches of steady states for $c_{Af} = 0.5$ kgm^{-3}; a) (upper left) a_1, b) (upper right) a_2, c) (lower left) a_3 and d) (lower right) enlargement of upper states of a_3 branch

The obtained results suggest that forcing on cascade to operate in the upper states may be realised not only by increasing the total residence time, but also by changing parameter x (for example, by way of setting the tree-way valve), especially in the case of higher concentration of substrate in the feed. Additionally, the width of upper states (Fig. 4e; region V in Fig. 2b) may provide protection against falling down to middle states under various values of total residence time. This indicates the practical application of such devices when the stream of the feed is changing during the process. On the other hand, further increasing the x parameter may result in biomass washout in reactors 1 and 3, and consequently, in such conditions, only reactor 2 can work effectively.

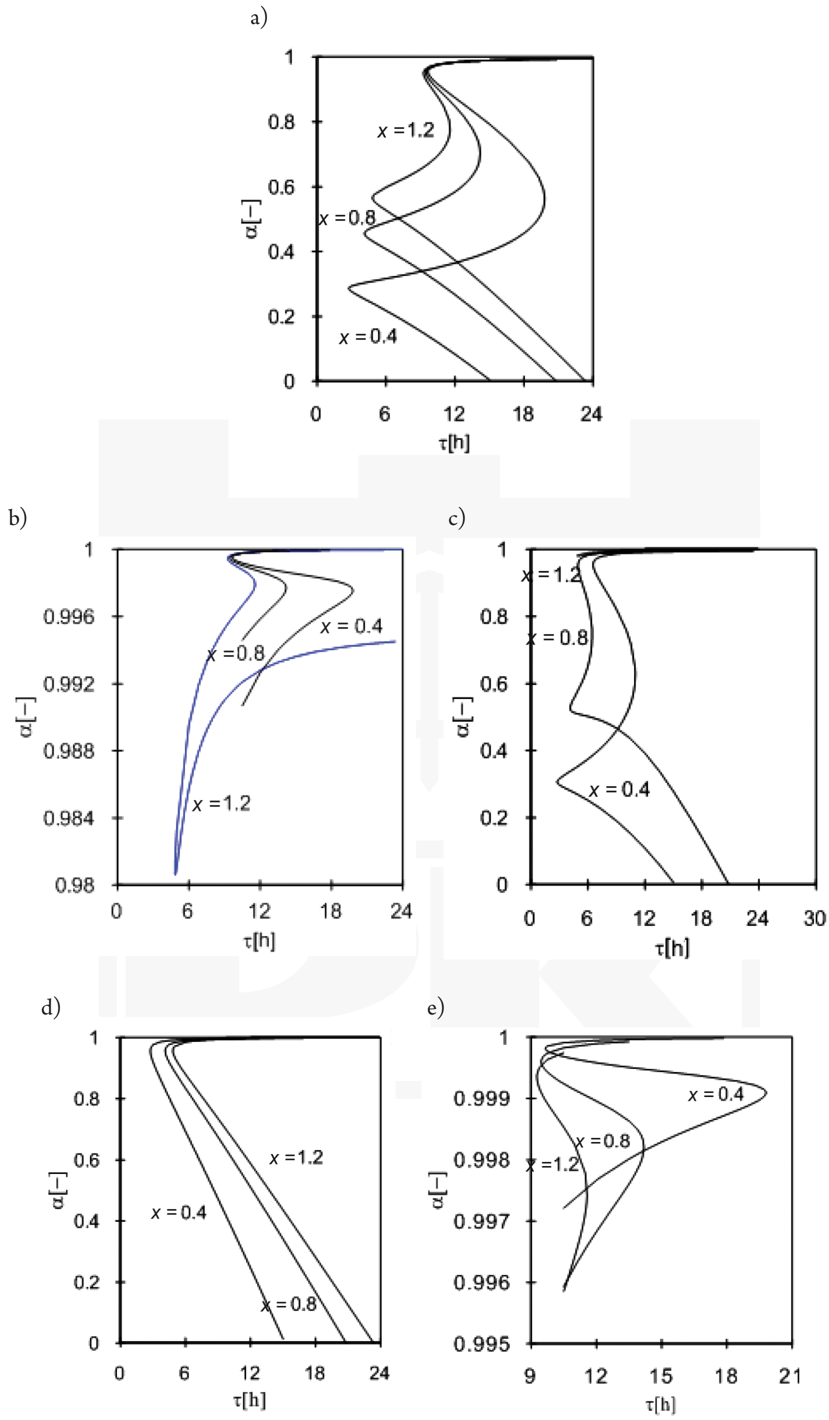

Fig. 4. Branches of steady states for c_{Af} = 1 kgm^{-3}; a) a_1 (first row), b) a_2 (second row, left), d) (third row, left) a_3 and enlargements of upper states for c) (second row, right) a_2; e) (third row, right) a_3

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