Computer simulation of transition modes in flow reactors considering the multistage and reactions non-perfectness

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Article Info

ABSTRACT

Due to the variety of reaction types and schemes in chemical-technological apparatuses, a general engineering methodology to assessing how the transient modes and reactions multi-stage act the kinetics in conditions of occurrence of moving reaction fronts in flow apparatuses has not yet been developed. The paper devotes to constructing the mathematical models for several important cases of the problem mentioned, namely: for theoretically study the kinetic dynamics of the conversion process in a three-stage chemical reaction with an autocatalytic first stage and the presence of a mass source of one of the components. An original mathematical model for describing the chemisorption dynamics at the initial stage of forming a moving reaction front in flow-through apparatuses has been developed. A special algorithm and numerical solution for the initial absorption period have been constructed, and appropriate computer simulation has been implemented. The significant influence of multistage on the formation and on stability types of stationary states has been established. Expressions to evaluate the characteristics of the emerging oscillatory modes have been obtained too. The results can be used to assess the influence of control parameters on the reaction front movement speed.

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1. INTRODUCTION

The study of transient regimes in flow reactors is crucial for calculating technological processes and designing technological schemes. These regimes influence the formation of various stationary operating modes in apparatuses. It has been established, that transient regimes in flow reactors significantly affect the total efficiency of the reactor and should be taken into account in the calculation methods of the technological process and equipment [1]-[3]. Exactly these transitional stages of the heat and mass transfer processes in reactors determine the formation of various stationary operating modes of through-flowing technological apparatuses [4]-[6]. Therefore, in order to select the optimal stationary operating regime that ensures the necessary efficiency of the process and the specified energy costs for its implementation, it is

necessary to have an adequate mathematical model that describes the features of transient modes in the apparatus [7], [8]. Transient modes also play a fundamental role in the development of a process control system [9]. It should be especially noted that the multistage nature of the chemical technological process, as well as thermodynamic non-perfectness, manifest themselves most clearly in non-stationary transient regimes [10], [11]. This is explained by the fact that multistage nature creates obvious prerequisites for the interaction of various kinetic mechanisms and competition of conversion rates at various stages of the kinetic scheme of the transformation of substances in the apparatus [12]-[14]. This topic is so broad and deep in terms of possible manifestations of various kinetic and thermal phenomena that at present many questions in this area remain open [15], [16].

Periodic operation modes of reactors of various types have attracted increased interest from researchers in recent years. A special place among the works devoted to these problems is occupied by the review [17]. This book provides an extensive introduction to a large number of literary sources. This opens up opportunities for an objective assessment of the results obtained recently. In particular, it has become obvious now that non-stationary operation modes can be considered as effective and little used yet resources to intensifying the processes of mass and heat transfer while simultaneously reducing specific energy consumption.

The authors note that although stationary modes of operation of chemical-technological apparatuses apparently remain the main industrial paradigm, it makes sense to deeply study possible and even necessary exceptions to this paradigm for the intensification of processes [17]. For example, a significant part of metallurgical processes occurs in non-stationary conditions. Stationary operation modes of reactor become impractical in many biochemical systems. Electrochemical processes have also used the advantages of the non-stationery modes for more than 60 years [17]. It is now a proven fact that periodic operation can often improve process productivity.

For example, methanol production is characterized by high productivity. Moreover, methanol is usually produced in fixed-bed reactors under steady-state conditions using a catalyst. At the same time, the possibility of a noticeable intensification of a methanol production reactor by forced periodic operation compared to operation in a steady-state mode is shown in the work [18]. The authors conducted a numerical study using a simplified model that describes a hypothetical 7-meter isothermal and isobaric fixed-bed reactor. The forced periodic mode is stimulated as a result of the harmonic action of square waves. Based on mathematical modeling, multi-objective optimization is performed for various sets of control parameters. As a result of the optimization, the achievable molar flow rate of methanol at the reactor outlet and the yield of methanol based on total carbon are quantitatively determined [18]. The main numerical methods used to solve this problem are based on the simultaneous approach with orthogonal collocation as a discretization. It was these studies that allowed the authors to conclude that it was advisable to organize the optimal mode by means of forced periodic operation with square waves. It was shown that periodic operation can provide theoretical improvements of up to 50% for the average molar flow rate of methanol at the outlet and improvements of up to 10% for the yield based on total carbon [18].

The paper is also devoted to the issues of methodology of calculation and design of reactors with the organization of forced periodic mode of operation in order to use nonlinear dynamics for intensification of reagent conversion [19]. In this paper, it is noted that the analysis of operation modes, the design of a technological scheme and choice of the optimal operation regime are associated with significant theoretical and engineering problems. The paper devotes to the mathematical aspects and new methods of regimes optimization which are based on the nonlinear frequency response (NFR) method. In this paper, the method of direct derivation of the NFR from the mathematical model of the main process has been considered. It is shown that in this case only qualitative conclusions can be made about the behavior of the process control characteristics. At the same time, this is not enough for the engineering method of calculating the intensity of transfer processes. Another approach developed in [19] is allowing for obtaining the data that open up opportunities for optimal design of the periodic mode of operation of chemical reactors. But this approach is suitable only for the case when oscillations of the process control parameters are induced, i.e. forced by some external source. This approach is allowing also for creating the NFR which can be suitable for quantitative assessment of the process characteristics and implementation of optimal design. However, the useful conclusions can be made only about induced, forced periodic modes. The article shows the results of applying a new approach to modeling a system of isothermal reactors of continuous mixing reactors in the process of carbon dioxide absorption. Comparison with experimental data shows the adequacy of the model and the effectiveness of the new approach.

Operating experience has shown that although catalytic reactors are irreplaceable in many industries, they do not meet the industry requirements in terms of productivity, stability and energy consumption. To solve such problems, reactors with an intensified process appear, which are most often based on alternative energy sources. The work provides an overview of known developments of catalytic reactors in terms of reactor types, catalyst bed structure and operating methods [20]. The review also presents

information on experimental data obtained at laboratory and pilot scales of various catalytic reactors. It is shown how the reactor geometry and the structure of the catalyst beds affect the hydrodynamics of multiphase catalytic processes. Ways to increase the process productivity and intensify heat and mass transfer are also described [20].

As the result of a literature sources analysis, it can be concluded that the problems of efficient use of non-stationary reactor operation modes, as well as the issues of optimizing their operation and reducing specific energy consumption, remain largely open and require further research. This especially concerns the issues of taking into account non-stationary modes that are not forcibly organized to intensify transfer processes [21]. The problems associated with the search for self-organizing modes at various stages and new possibilities for a radical increase in the intensity of transfer processes with moderate additional energy costs remain very relevant too.

The main objective of this work is to develop mathematical models and conduct computer simulation for processes using the example of a reaction that can be used as a model of many technological industrial processes associated with autocatalysis. The novelty and scientific contribution of the submitted work lie in that these aspects of modeling have been studied applying to autocatalytic reactions of two types that are often found in various technological schemes of real industrial processes [22], [23]. The original mathematical model for describing chemisorption dynamics at the initial stage of formation of a moving reaction front in through-flowing apparatuses has also been carried out [24]. The special algorithm and numerical solution of the problem for the absorption initial period have been constructed, and appropriate computer simulation has been implemented.

2. THE COMPREHENSIVE THEORETICAL BASIS

This section devotes to analyzing some important cases in arising the transition modes in flow reactors.

2.1. Impact of multistage process nature

Let's consider the following model reaction scheme, in which the main reagents are components X and Y, the intermediate ones are A, C and the first stage is autocatalytic in nature [25].

$$X + Y \xrightarrow{k_1} X \tag{1}$$

$$X \xrightarrow{k_2} A \tag{2}$$

$$Y \xrightarrow{k_3} C \tag{3}$$

Here k_1, k_2, k_3 are the kinetic rate constants for the process stages.

Next, the case of continuous supply of a component Y to the reactor at a rate of q has been considered. Then the system of kinetic equations for the main components (see (1), (2), (3)) can be written as:

$$\frac{dX}{dt} = k_1 XY - k_2 X, \; \frac{dY}{dt} = q - k_1 XY - k_3 Y \tag{4}$$

thus, the set of stationary states can be described as a result of solving the system (4) of algebraic equations:

$$k_1 XY - k_2 X = 0, \; q - k_1 XY - k_3 Y = 0 \tag{5}$$

From (5) it is follows, due to the autocatalytic properties of the component X, the following stationary point is stable:

$$X_{00} = 0; \; Y_{00} = \frac{q}{k_3} \tag{6}$$

Besides, this stationary point (6) is also the only one, provided that the component Y entry rate is small, and it satisfies the following inequality:

$$q < q^* = \frac{k_2 k_3}{k_1} \tag{7}$$

As the entry rate increases above the critical value described by inequality (7), another stationary state arises in the system.

$$X_{01} = \frac{qk_1 - k_2k_3}{k_1k_2}; \quad Y_{01} = \frac{k_2}{k_1} \tag{8}$$

So, when $q > \frac{k_2k_3}{k_1}$ the stationary point (6) becomes unstable. And the new emerging stationary state (8), on the contrary, is stable. The corresponding stationary point can be either a node or a stable focus. In this case, a damped oscillatory transient regime occurs in the system. A detailed analysis of the modes based on known techniques in this case gave the following results.

If $\frac{k_3}{k_2} \geq 1$, then stationary point (8) under $q > \frac{k_2k_3}{k_1}$ is a stable node. Therefore, the oscillatory mode does not occur. If $\frac{k_3}{k_2} < 1$ and $q > \frac{k_2k_3}{k_1}$, then the following relation always is true.

$$q^* < \frac{2k_2^2}{k_1}\left[1 - \sqrt{1 - \frac{k_3}{k_2}}\right] \tag{9}$$

It follows that when the reagent Y supply rate exceeds the critical value q^* (see (9)) and provided the inequality $\frac{k_3}{k_2} < 1$ that within a certain range of reagent supply rates a transient oscillatory mode will occur. The appropriate range reads,

$$q_1 < q < q_2 \tag{10}$$

here:

$$q_1 = \frac{2k_2^2}{k_1}\left[1 - \sqrt{1 - \frac{k_3}{k_2}}\right], \quad q_2 = \frac{2k_2^2}{k_1}\left[1 + \sqrt{1 - \frac{k_3}{k_2}}\right] \tag{11}$$

For the oscillatory transition mode that occurs at the bounds (10) after the bifurcation (11), the frequency of the occurring oscillations and the logarithmic attenuation decrement can be determined as (12).

$$\omega = \sqrt{\frac{2q}{k_3} - \frac{2k_2k_4}{k_1k_3} - \frac{k_3k_4^2}{4}}, \quad \nu = -\frac{k_4}{2} \tag{12}$$

Thus, the main characteristics of the induced oscillations can be calculated from (12).

2.2. Impact of the process non-perfectness
This section is devoted to the analysis of the autocatalytic reaction of the following type:

$$A + X \underset{k_2}{\overset{k_1}{\rightleftharpoons}} 2X \tag{13}$$

In an ideal system, the following relationship is valid for the chemical potential of the reaction product [26]:

$$\mu = \mu^* + RT \ln X \tag{14}$$

were μ^* - standard value of chemical potential; R - gas constant; T - temperature.
In contrary to (14) the following expression for the chemical potential of the reaction (13) product in a dilute binary system is valid:

$$\mu = \mu^* + RT \ln X + \omega_{AX}(1 - X)^2 \tag{15}$$

where,

$$\omega_{AX} = \kappa[2\varepsilon_{AX} - (\varepsilon_{AA} + \varepsilon_{XX})] \tag{16}$$

In formulas (15), (16) the following notations are used: $\varepsilon_{AX}, \varepsilon_{AA}, \varepsilon_{XX}$ - energies of interaction between reagents A and X, A and A, X and X molecules respectively; κ- parameter dependent on the liquid state model used. Since the solution is taken diluted, it can be assumed that $X \ll 1$. Then instead of (23) it can be written an approximate equality:

$$\mu = \mu^* + RT \ln X + \omega_{AX}(1 - 2X) \tag{17}$$

In accordance with the provisions of the thermodynamics of dilute solutions, the diffusion coefficient is dependent on the value of the derivative of the chemical potential (17) with respect to concentration:

$$\frac{\partial \mu}{\partial X} = \frac{RT}{X} - 2\omega_{AX} \tag{18}$$

from this it follows,

$$D = D_i(1 - 2\omega_{AX}X) \tag{19}$$

where D - the diffusion coefficient in the real system; D_i - value of the diffusion coefficient for an ideal system. Using the self-similar variable technique applying to (18), (19), a kinetic equation can be reduced to the system (20). The corresponding system of first-order equations takes the form:

$$\begin{cases} X' = Y, \\ Y' = \frac{V-c}{D_i(1-2\omega_{AX}X)}Y + \frac{2\omega_{AX}}{1-2\omega_{AX}X}Y^2 - \frac{f(X)}{D_i(1-2\omega_{AX}X)} = 0 \end{cases} \tag{20}$$

here,

$$f(X) = k_1 AX - k_2 X^2 \tag{21}$$

From (20), (21) it follows there are two possible stationary states in the reactor:

$$X_{01} = 0; X_{02} = A\frac{k_1}{k_2} \tag{22}$$

The Jacobians of the linearized system in the vicinity of each of the stationary points (22) look as follows:

$$J_1 = \begin{pmatrix} 0 & 1 \\ -\frac{k_1 A}{D_i} & \frac{V-c}{D_i} \end{pmatrix}, J_2 = \begin{pmatrix} 0 & 1 \\ \frac{k_1 A}{D_i(1-\gamma)} & \frac{V-c}{D_i(1-\gamma)} \end{pmatrix} \tag{23}$$

here V - stream velocity; c - phase velocity;

$$\gamma = 2\omega_{AX}\frac{k_1}{k_2}A \tag{24}$$

Since for dilute solutions $\omega_{AX} \ll 1$, the following inequality applying (23), (24) is valid [26].

$$\gamma < 1 \tag{25}$$

The analysis carried out convincingly shows that the thermodynamical deviation from mixture non-perfectness does not significally act the stationary regimes character [26]. At the same time, the initial rate of moving wave front may differ significantly from that calculated for perfect mixtures. With the help of Taylor series expansion under the small values of the correction parameter γ (25), the relation for phase velocity can be reduced to the form [27].

$$c_{0r} = c_0 + \gamma\sqrt{k_1 D_i A} \tag{26}$$

Where c_0 is the phase velocity of moving waves in the perfect system?

$$c_0 = |V - 2\sqrt{k_1 DA}| \tag{27}$$

The analysis of considered model (26), (27) demonstrates that the rate of reagents supply in chemical reactors can be useful not only for control of the reactor productivity, but can also qualitatively change the set of stationary and transient modes. Such changes can be associated with the thermal operating conditions first at all.

3. METHOD

The method for researching the behavior of operation modes especially in relation to chemisorption dynamics in reactors with a moving reaction front has been carrying out. This section devotes to the main method describing applying to the regularities in mass transfer dynamics in the cases of moving reaction fronts. The problem of calculating the time of formation and the movement rate of the reaction front for absorption, accompanied by an instantaneous irreversible chemical reaction, has been considered in [27].

$$A + B \rightarrow E \tag{28}$$

The basic position of the model is the assumption that reagent B is uniformly distributed in the incoming liquid film. Unlike reagent B, reagent A is uniformly distributed in the gas phase and diffuses to the liquid-gas interface. Then three main stages of the process can be determined [27].

At the first stage, namely, in the period $0 < t < t^*$, reagent A has not yet reached the interface. At the same time, the concentration of component B decreases. Therefore, it can be considered that the reaction front is at the interface. The second stage of the process begins at the moment $t = t^*$. At this moment, the maximum decrease in the concentration of component B at the gas-liquid interface occurs, and an instantaneous chemisorption reaction begins. As a result of this reaction, reagent E is formed. At the end of the second stage of the process, the reaction front becomes mobile and begins to move deep into the liquid phase.

The third stage begins at $t > t^*$. At this stage, three zones can be distinguished by the layer depth. The first zone is the physical absorption zone; the second zone is characterized by the presence of a moving reaction front. In this zone, the intensive formation of the reaction product occurs. The third zone is characterized by the diffusion of the active reagent B and the resulting reaction product E. Thus, at $t > t^*$, the reaction front becomes mobile. The problem posed does not have an analytical solution at this stage [26], [27]. For the finite difference discretization of the diffusion (29), an appropriate modification of the standard Crank-Nicolson schemes is implemented [28]. In these equations a, b and δ are the parameters of the non-uniform mesh, u is concentration of a component at a point according to a numerical model.

In order to find the run coefficients from the condition on the right boundary, the expression (29), (30) were rewritten as follows.

$$bu_{i+1}^{j+1} - u_i^{j+1}(a+b) + au_{i-1}^{j+1} + bu_{i+1}^{j} - u_i^{j}(a+b) + au_{i-1}^{j} = \delta(u_i^{j+1} - u_i^{j}) \tag{29}$$

$$bu_{i+1}^{j+1} - u_i^{j+1}(a+b+\delta) + au_{i-1}^{j+1} = -bu_{i+1}^{j} + u_i^{j}(a+b-\delta) - au_{i-1}^{j} \tag{30}$$

Here a, b - non-uniform mesh parameters; u_i^{j} −concentration of components. The obtained numerical mathematical model (29), (30) has been solved by the run method according to the scheme [26]. Figure 1 shows a code fragment of the run method in the Mathcad engineering package. The use of this method ensures the convergence of results and allows for selecting the calculation step that is necessary to achieve the specified numerical error [29].

Figure 1. Code fragment by the run method in Mathcad system

4. DISCUSSION OF THEORETICAL PREREQUISITES AND RESULTS OF NUMERICAL SIMULATION

4.1. Preliminary discussion of the main model

In the work [30] a model of the chemisorption process in a system with a moving reaction front is proposed. However, this model does not take into account the influence of the reaction product on the rate of diffusion of reagents in the liquid layer at $t < t^*$. At the same time, there is no reason to believe that such an influence is really insignificant during the exhaustion of the active component in the vicinity of the interphase boundary. The following relations accounting the mentioned influence read:

$$j_B = -D_{BB}\frac{\partial c_B}{\partial x} - D_{BE}\frac{\partial c_E}{\partial x}, j_E = -D_{EB}\frac{\partial c_B}{\partial x} - D_{EE}\frac{\partial c_E}{\partial x}. \tag{31}$$

At the initial period of the absorption process (31) the reaction front still coincides with the interphase boundary and sources of mass in the liquid layer are absent. In this case, in the depth of the liquid phase at $x > 0$ (here $x = 0$ is the phase interface), the laws of conservation of mass of the components must be satisfied. The solution of system (31) with the corresponding boundary conditions is obtained using the Laplace transform. The reaction front becomes mobile at the moment of exhaustion of the active reagent B near the interphase surface [27].

$$t^* = \frac{c_{B\infty}^2 \pi (R_2 - R_1)^2}{4\alpha^2 c_{A\infty}^2 \left(\frac{2T_2 R_1 + T_1 R_2}{\sqrt{S_2}} - \frac{2T_2 + T_1}{\sqrt{S_1}}\right)} \tag{32}$$

For times greater than t^*, the analytical solution to the problem is unknown [31], [17].

4.2. Discussion of the numerical solution of the problem at times outside the initial period, i.e by $t > t^*$

In this work the possible influence of a concentration jump during the transition through the concentration front on the hydrodynamic picture was not taken into account. This issue is subject to special study in cases where the physical characteristics of a liquid or gas significantly depend on the concentrations of impurities. Some typical results of numerical experiments are shown in Figure 2. Legend: 1-B=6 mol/m³, 2-B=7 mol/m³, 3-B=8 mol/m³, 4-B=9 mol/m³, 5-B=10 mol/m³.

The initial velocity V_1 of the moving reaction front depends on the step along the longitudinal coordinate Δx_1. This step this step was chosen so as to satisfy the condition (33).

$$V_0 < V_1 < V_2 \tag{33}$$

The second stage begins at the penetration time moment $t = t_p$. The movement low of the reaction front in this stage can be described by the film model [28].

The principal result of the numerical experiment is the conclusion that the reaction front rate quickly increases in the initial period from $t > t^*$. And then, after a certain moment, this rate begins to decrease with tending to zero. In Figure 2, these two periods are visible. During the first period up to the moment $t = t_p$, which corresponds to the maximum velocity of the reaction front, the evaluation of the characteristic depth of the reaction front penetration has been obtained.
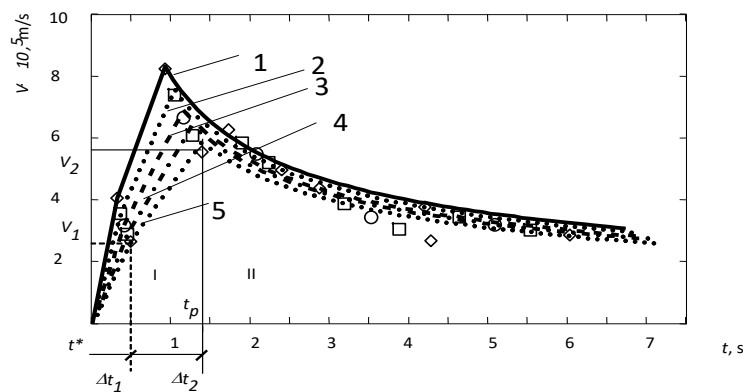

Figure 2. Reaction front velocity V at absorption time $t>t^*$

5. CONCLUSION

The goal of the work has been achieved, as the mathematical model that made it possible to theoretically study the kinetic dynamics of the conversion process in a three-stage chemical reaction with an autocatalytic first stage and the presence of a mass source of one of the components has been carried out. As the result, forecast made about significant influence of multistage on the formation of stationary states of transformation processes, types of stability have been identified, and unstable states and bifurcation points of regimes in the space of control parameters have been found. Expressions were obtained to evaluate the characteristics of the emerging oscillatory modes. A mathematical model of chemisorption dynamics at the stage of formation of a moving reaction front and computer simulation on the base of the novel model and special numerical algorithm have been carried out.

The results obtained can be used for assessment of the influence of process parameters on the velocity of movement of the reaction front. As a result of numerical experiment, it is possible to determine characteristic spatial and temporal scales of the film model. It means, that without a priori setting of the film thickness an estimation of this value can be obtained as characteristic values of the depth of penetration of component A into the liquid phase of the absorbent at the first stage of the reaction front advancement.

Of course, the direct results of this work can be more or less reliably used to analyze those processes whose kinetic scheme is adequately described by the model schemes considered in the work. However, the methods of analysis used in the work can be adapted to other model schemes. This work has yet to be completed by the authors. In addition, it is necessary to analyze in more detail a larger volume of experimental data and reports on the operation of reactors in non-stationary modes.

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