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ИЗВЕСТИЯ

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Қазақстан Республикасы Ұлттық ғылым академиясы "ҚР ҰҒА Хабарлары. Геология және техникалық ғылымдар сериясы" ғылыми журналының Web of Science-тің жаңаланған нұсқасы Emerging Sources Citation Index-те индекстелуге қабылданғанын хабарлайды. Бұл индекстелу барысында Clarivate Analytics компаниясы журналды одан әрі the Science Citation Index Expanded, the Social Sciences Citation Index және the Arts & Humanities Citation Index-ке қабылдау мәселесін қарастыруда. Webof Science зерттеушілер, авторлар, баспашылар мен мекемелерге контент тереңдігі мен сапасын ұсынады. ҚР ҰҒА Хабарлары. Геология және техникалық ғылымдар сериясы Emerging Sources Citation Index-ке енуі біздің қоғамдастық үшін ең өзекті және беделді геология және техникалық ғылымдар бойынша контентке адалдығымызды білдіреді.

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MODELING OF DYNAMICAL REACTION-DIFFUSION SYSTEMS WITH MULTISTAGE AND NON-PERFECT KINETICS

Abstract. The paper deals with the problems of dynamical models describing reaction-diffusion systems characterizing by the multistage and non-perfect kinetics. The main types of dynamical behavior of such systems using two typical examples have been considered. As a result of the research it was concluded that multistage and non-perfect kinetics can strongly influence on the reactor regimes and change their main characteristics. It wasalso concluded that non-perfect kinetics in the case of high diluted solutions doesn't change types of rest points and reactor regimes. However, velocity of wave front which generates from transient oscillatory regimes differs from the velocity of wave front in a perfect system.

Concrete values of regimes characteristics have undergone changes too. It was shown that the rate of reagents supply not only controls an output of the reactor but also can essentially change a set of stationary and transition process regimes. Usually engineers connect such transformations with heat phenomena. The mentioned above factors can also cause regime transitions. In addition the set of parameters controlling the regime stability and describing the system bifurcations has been obtained.

The main types of possible dissipate structures caused by these factors as well as cases of their formation have been also determined. Besides, transition regimes are determined by a system non-linearity. However in the case of strong solutions the situation may be different. This problem needs an additional study. The results of the research are feasibly to be useful for calculating the intensity of mass transfer processes in chemical reactors.

Key words: dissipate structures,multistage kinetics, non-perfect systems, reaction-diffusion systems.

Introduction. Multistage kinetics and non-perfectness of reaction-diffusion systems have an essential influence on the process regime in chemical reactors [1]. It is well-known that multistage kinetics can stimulate the origin of multiplicity of stationary points in system dynamics. Besides, chemical oscillations are observed only in the multistage reaction-diffusion systems [2].

Non-perfectness is also very important aspect that can play an essential role under generating dynamical regimes in the point of view of chemical thermodynamics [3]. And concrete values of regimes characteristics can undergo changes too.

However engineers often do not give due attention to these aspects of chemical processes and its impact on the apparatuses design. They usually connect such transformations only with heat phenomena. But the mentioned above factors can also cause regime transitions.

In our work this problem has been theoretically investigated and illustrated by means of two model auto-catalytic reactions as examples.

Model systems with multistage kinetics. Firstly we consider the following model scheme with the main reagents X, Y and intermediate products A, C, despite the first stage is supposed to be an auto-catalytic reaction [3]:

$$X + Y \xrightarrow{k_1} X, \quad X \xrightarrow{k_2} A, \quad Y \xrightarrow{k_3} C, \tag{1}$$

where k_1, k_2, k_3 are the reactions rate constants.

Let's assume that the component Y enters the reactor continuously with constant supply rate q, and the reagent X is the initial priming-tube.

Thus the system of kinetic equations for main reagents reads [4]:

$$\begin{aligned} \frac{dX}{dt} &= k_1 XY - k_2 X, \\ \frac{dY}{dt} &= q - k_1 XY - k_3 Y. \end{aligned} \tag{2}$$

Here $X \geq 0$ and $Y \geq 0$ denote concentrations of reagents X and Y.

Provided the rate q satisfying the inequation

$$q < \frac{k_2 k_3}{k_1} \tag{3}$$

there is the only stable rest point of the system (2)

$$X_{01} = 0; \quad Y_{01} = \frac{q}{k_3}. \tag{4}$$

But when this rate exceeds the critical value

$$q > q^* = \frac{k_2 k_3}{k_1} \tag{5}$$

the system acquires yet another rest point:

$$X_{02} = \frac{qk_1 - k_2 k_3}{k_1 k_2}; \qquad Y_{02} = \frac{k_2}{k_1}. \tag{6}$$

Jacobians of the linearized system of kinetic equations at the rest points have the following

$$J_{01} = \begin{pmatrix} -k_2 + \dfrac{k_1 q}{k_3} & 0 \\ -\dfrac{k_1 q}{k_3} & -k_3 \end{pmatrix}, \tag{7}$$

$$J_{02} = \begin{pmatrix} 0 & \dfrac{qk_1 - k_2 k_3}{k_2} \\ -k_2 & -\dfrac{qk_1}{k_2} \end{pmatrix}. \tag{8}$$

Provided $q > q^*$ the rest point (4) becomes unstable. And the springing up rest point (6) becomes stable on the contrary and it has a type of stable node or stable spiral.

The regimes analysis gives the following results:

1) for $(k_3/k_2) \geq 1$ at any q the rest point (6) is a stable node, and oscillations donot exist;

2) for $(k_3/k_2) < 1$ at q exceeding the critical value q^* rest point (6) can be a spiral.

At $(k_3/k_2) < 1$ we have

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

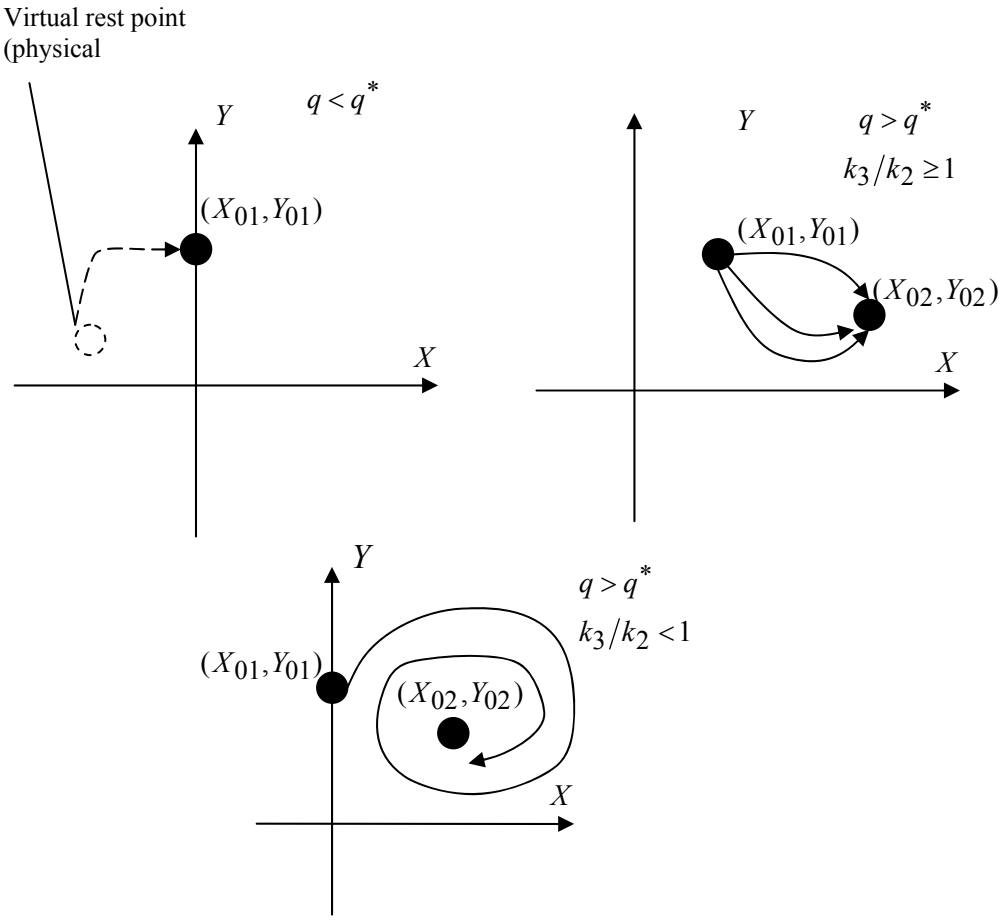
From this it follows that provided $(k_3/k_2) < 1$ and $q > q^*$ the rest point (6) is a stable spiral, and appropriate transition regime goes on in the form of oscillations at the rate range

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

where

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

$$q_2 = \frac{2k_2^2}{k_1}\left[1 + \sqrt{1 - \frac{k_3}{k_2}}\right]. \tag{12}$$



Phase curves near the rest points of the system (2)

Thus the system has the control parameter

$$\alpha = \frac{k_3}{k_2}. \tag{13}$$

The value $\alpha = \alpha^* = 1$ is the bifurcation point, and for the transition regime we can obtain the frequency of oscillations ω and the logarithmic fading decrement ν:

$$\omega = \sqrt{\frac{2q}{k_3} - \frac{2k_2k_4}{k_1k_3} - \frac{k_3k_4^2}{4}}, \tag{14}$$

$$\nu = -\frac{k_4}{2} \tag{15}$$

The second example is the auto-catalytic reaction of the following type [2, 3]:

$$A + X \underset{k_2}{\overset{k_1}{\rightleftarrows}} 2X + C\,. \tag{16}$$

In the perfect thermodynamic system the following relation is true

$$\mu = \mu^* + RT \ln X\,, \tag{17}$$

where μ is a chemical potential and μ^* - its standard value, R is gas constant, T is a temperature.

Impact of system non-perfectness. Let's consider the case of non-perfect reaction-diffusion system, where the chemical potentials of reagents read [5].

$$\mu = \mu^* + RT \ln X + \omega_{AX}(1 - X)^2\,. \tag{18}$$

Here

$$\omega_{AX} = \kappa[2\varepsilon_{AX} - (\varepsilon_{AA} + \varepsilon_{XX})], \tag{19}$$

and ε_{AX}, ε_{AA}, ε_{XX} are energies of interaction between molecules of reagents, κ is a parameter depending on the model of liquid state [6-8].

Supposing $X << 1$ we obtain the following approximate relation

$$\mu = \mu^* + RT \ln X + \omega_{AX}(1 - 2X). \tag{20}$$

According to thermodynamics of diluted solutions, the diffusion coefficients determine by the derivatives of chemical potentials over the concentrations [9].

Thus we obtain:

$$\frac{\partial \mu}{\partial X} = \frac{RT}{X} - 2\omega_{AX} = \frac{RT}{X}(1 - 2\omega_{AX} X), \tag{21}$$

From this it follows

$$D = D_i(1 - 2\omega_{AX} X), \tag{22}$$

where D_i is the diffusion coefficient in perfect system, D is the one in a real system [10-12].

And so, the mass transfer equation for the reaction (15) proceeding in a tubular through-reactor can be written as follows

$$\frac{\partial X}{\partial t} + q\frac{\partial X}{\partial z} = \frac{\partial}{\partial z}\left(D_i(1 - 2\omega_{AX} X)\frac{\partial X}{\partial z} \right) + f(X), \tag{23}$$

where

$$f(X) = k_1 AX - k_2 X^2\,. \tag{24}$$

Using method of an auto-model variable the equation (23) can be reduced to the following ordinary differential equation [13]

$$\frac{d^2 X}{ds^2} - \frac{q - c}{D_i(1 - 2\omega_{AX} X)}\frac{dX}{ds} - \frac{2\omega_{AX}}{1 - 2\omega_{AX} X}\left(\frac{dX}{ds}\right)^2 + \frac{f(X)}{D_i(1 - 2\omega_{AX})} = 0\,, \tag{25}$$

where $s = x - ct$, c is a phase velocity or a velocity of wave front.

Equations of the appropriate dynamical system read

$$\begin{cases} \dfrac{dX}{dt} = Y, \\ \dfrac{dY}{dt} = \dfrac{q-c}{D_i\left(1-2\omega_{AX}X\right)}Y + \dfrac{2\omega_{AX}}{1-2\omega_{AX}X}Y^2 - \dfrac{f(X)}{D_i\left(1-2\omega_{AX}X\right)} = 0 \end{cases} \tag{26}$$

There are two rest points of the system

$$X_{01} = 0, \quad X_{02} = A\frac{k_1}{k_2}. \tag{27}$$

Jacobians of the linearized system (26) at the rest points (27) read

$$J_{01} = \begin{pmatrix} 0 & 1 \\ -\dfrac{k_1 A}{D_i} & \dfrac{q-c}{D_i} \end{pmatrix}, \tag{28}$$

$$J_{02} = \begin{pmatrix} 0 & 1 \\ \dfrac{k_1 A}{D_i(1-\gamma)} & \dfrac{q-c}{D_i(1-\gamma)} \end{pmatrix}. \tag{29}$$

where

$$\gamma = 2\omega_{AX} A\frac{k_1}{k_2}. \tag{30}$$

As for diluted solutions $\omega_{AX} << 1$ the following inequation is correct

$$\gamma < 1. \tag{31}$$

From detail analysis which is analogous with the analysis of system (2) we conclude that non-perfect kinetics in the case of high diluted solutions does not change types of rest points and reactor regimes. At the same time, concrete values of regimes characteristics have undergone changes [14-17].

Particularly, the velocity of wave front which generates from transient oscillatory regimes differs from the velocity of wave front in a perfect system [18].

The appropriate relation reads

$$c_{0r} = c_0 + \gamma\sqrt{k_1 D_i A}\ . \tag{32}$$

Here c_0 is the wave front velocity calculated for the perfect system:

$$c_0 = \left|q - 2\sqrt{k_1 DA}\right|, \tag{33}$$

and $\gamma < 1$ is the special amendment coefficient for which we obtain the following relation

$$\gamma = 2\omega_{AX}\frac{k_1}{k_2}A. \tag{34}$$

Conclusion. It can be concluded that rate of reagents supply not only controls an output of the reactor but also can essentially change a set of stationary and transition process regimes. Usually engineers connect such transformations with heat phenomena [19]. At the same time the mentioned above factors can also cause regime transitions.

As regards the non-perfection of systems its influence for high diluted solutions manifests only in increasing the wave front velocity under transition regimes [20]. Incidentally, transition regimes-themselves are determined by a system non-linearity. However in the case of strong solutions the situation may be different. This problem needs an additional study [21].

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ДИНАМИКАЛЫҚ РЕАКЦИЯЛЫҚ-ДИФФУЗИЯЛЫҚ ЖҮЙЕЛЕРДІ КӨПСАТЫЛЫ ЖӘНЕ ИДЕАЛДЫ ЕМЕС КИНЕТИКАМЕН МОДЕЛЬДЕУ

Аннотация. Жұмыс көп сатылы және идеалды емес кинетикамен сипатталатын реакциялық-диффузиялық жүйелерді сипаттайтын динамикалық үлгілердің мәселелеріне арналған. Осындай жүйелердің динамикалық мінез-құлқының негізгі түрлері екі типтік мысалды қолдану арқылы қарастырылды. Зерттеудің нәтижесінде көп сатылы және идеалдық емес кинетика реактор режимдеріне қатты әсер етуі және олардың негізгі сипаттамаларын өзгертуі мүмкін деген қорытынды жасалды. Сондай-ақ, жоғары дәрежелі сұйылтылған ерітінділер жағдайында идеалды емес кинетика тыныштық нүктелері мен реактор режимдерінің түрлерін өзгертпейді деген қорытынды жасалды. Дегенмен, уақытша ауытқу режимдерінен туындайтын толқындық майдан (фронт) жылдамдығы толқындық майдан (фронт) жылдамдығынан идеалды жүйеде ерекшеленеді. Режимдердің сипаттамаларының нақты мәндері де өзгерді. Реагенттердің берілу жылдамдығы тек реактордың шығуын бақылап қана қоймай, сонымен қатар стационарлық және өтпелі процестер режимдерінің жиынтығын айтарлықтай өзгерте алатындығы көрсетілді. Әдетте инженерлер мұндай өзгерістерді жылулық құбылыстармен байланыстырады. Жоғарыда аталған факторлар өтпелі режимдерді тудыруы мүмкін. Режимнің тұрақтылығын басқаратын және жүйенің бифуркациясын сипаттайтын параметрлер жиынтығы да алынды. Осы факторларға байланысты мүмкін диссипативті құрылымдардың негізгі түрлері, сондай-ақ оларды қалыптастыру жағдайлары анықталған. Сонымен қатар, өтпелі режимдер жүйенің сызықтық еместігі арқылы анықталады. Алайда, концентрацияланған ерітінділер болған кезде, жағдай басқаша болуы мүмкін. Бұл мәселе қосымша зерттеуді талап етеді. Зерттеу нәтижелері химиялық реакторларда жаппай тасымалдау процестерінің қарқындылығын есептеу үшін пайдалы болуы мүмкін.

Түйін сөздер: диссипативті құрылымдар, көп сатылы кинетика, идеалды емес жүйелер, реакциялық-диффузиялық жүйелер.

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МОДЕЛИРОВАНИЕ ДИНАМИЧЕСКИХ РЕАКЦИОННО-ДИФФУЗИОННЫХ СИСТЕМ С МНОГОСТАДИЙНОЙ И НЕИДЕАЛЬНОЙ КИНЕТИКОЙ

Аннотация. Работа посвящена проблемам динамических моделей, описывающих реакционно-диффузионные системы, характеризующиеся многосдадийной и неидеальной кинетикой. Рассмотрены основные типы динамического поведения таких систем с использованием двух типичных примеров. В результате исследования был сделан вывод о том, что многостадийная и неидеальная кинетика может оказывать сильное влияние на режимы реактора и изменять их основные характеристики. Также было сделано заключение о том, что неидеальная кинетика в случае сильно разбавленных растворов не меняет типов точек покоя и режимов реактора. Однако скорость фронта волны, которая возникает из переходных колебательных режимов, отличается от скорости фронта волны в идеальной системе. Конкретные значения характеристик режимов также претерпели изменения. Было показано, что скорость подачи реагентов не только контролирует выход реактора, но также может существенно изменить набор режимов стационарного и переходного процессов. Обычно инженеры связывают такие преобразования с тепловыми явлениями. Указанные выше факторы также могут вызывать переходные режимы. Был получен также набор параметров, управляющих стабильностью режима и описывающих бифуркации системы. Определены также основные типы возможных диссипативных структур, вызванные этими факторами, а также случаи их образования. Кроме того, переходные режимы определяются системной нелинейностью. Однако в случае концентрированных растворов ситуация может быть иной. Эта проблема нуждается в дополнительном исследовании. Результаты исследования могут быть полезны для расчета интенсивности процессов массопереноса в химических реакторах.

Ключевые слова: диссипативные структуры, многостадийная кинетика, неидеальные системы, реакционно-диффузионные системы.

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