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Sensitivity analysis of a direct problem solution to kinetic parameters changes in a given range

Análisis de sensibilidad de una solución de problema directo a cambios en los parámetros cinéticos en un rango dado

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ABSTRACT

The paper shows a technique of researching the direct kinetic problem sensitivity to the variation of the kinetic parameters within a given range. This technique is based on the use of the computing device of the interval analysis. The direct problem solution in the conditions of kinetic parameter uncertainty was received by the interval method of the solution of a Cauchy problem for differential equations system. The interval characteristics received during this method application were used for the research of reagents and product concentration sensitivity about kinetic parameters of a mathematical model of industrially important reaction.

Keywords: Chemical kinetics, direct kinetic problem, interval analysis, sensitivity of decision.

RESUMEN

El artículo muestra una técnica de investigación de la sensibilidad del problema cinético directo a la variación de los parámetros cinéticos. Esta técnica se basa en el uso del dispositivo informático del análisis de intervalos. La solución del problema directo en las condiciones de incertidumbre de los parámetros cinéticos se recibió mediante el método de solución de intervalo de un problema de Cauchy para el sistema de ecuaciones diferenciales. Las características de intervalo recibidas durante la aplicación de este método se usaron para la investigación de reactivos y sensibilidad de concentración de productos en relación con reacciones de importancia industrial.

Palabras clave: Análisis de intervalos, cinética química, problema cinético directo, sensibilidad de la decisión.

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1. INTRODUCTION

Mathematical modeling of a chemical process begins with a kinetic model. The kinetic model determines the reaction rate. The kinetic model includes the reaction mechanism, the speed equations of individual stages, kinetic parameters (constants of the speed and activation energy) and some simplifying provisions about the role of individual stages. Changes in concentrations of substances can be described by kinetic curves of flow or formation of reaction reagents and products. To construct such dependencies, it is necessary to solve a direct kinetic problem. The main task of chemical kinetics is to calculate the composition of a multicomponent reacting mixture and the reaction rate.

The paper studies the influence of uncertainty in kinetic parameters on the results of solving the direct problem of chemical kinetics. Kinetic data are represented in intervals and are considered as objects of interval analysis. A modified method of interval sensitivity analysis was used to solve the direct kinetic problem (Shary: 2013; Mustafina et al.: 2017, pp. 805-815; Khaydarov et al.: 2012, pp. 112-114; Pakdel & Ashrafi: 2019; Annía, Villalobos, Romero, Ramírez & Ramos: 2018). The main idea of this method is to analyze partial derivatives of the parameter solution. For the implementation of this method, the technique of interval analysis is used.

In work (Shary: 2013) it is shown that the problem of not uniqueness of the solution of the inverse problem of determination of kinetic parameters can be solved by reduction of the generally accepted statement of the given problem, to a kind according to which the area becomes the solution, arbitrary variation of kinetic constants of speeds in which the demanded quality of the description of experiment is kept. One of the approaches to determine the desired area is based on the application of the computational apparatus of interval analysis to calculate the uncertainty intervals of kinetic parameters (Mustafina et al.: 2017, pp. 805-815; Ramírez, Lay, Avendaño y Herrera: 2018; Rincón, Sukier, Contreras y Ramírez: 2019).

2. MATERIAL AND METHODS

The mathematical model of a chemical reaction is a system of ordinary differential equations of the first order with given initial conditions:

$$\frac{dx_i}{dt} = f_i(t, \mathrm{x}, \mathrm{k}), t \in [0;T]$$
$$x_i(0) = x_i^0 \; i = \overline{1,n}, \tag{1}$$

,,

Where x_i – concentration of the *i*-th component (molar shares), *n* – the number of substances, k – vector of kinetic constants of reaction speeds of *m* dimension, *T* – reaction course time. The system of the equations with entry conditions (1) represents the definition of Cauchy problem for ordinary differential equations systems.

In some cases, there is a need for the direct problem solution in the conditions of initial physical and chemical information uncertainty (Mustafina et al.: 2017, pp. 805-815). We will understand representation of speeds constants in an interval form as the partial uncertainty in kinetic data (Khaydarov et al.: 2012, pp. 112-114). Thus we will present the speeds constants vector in the form (Kalmykov: 1986).

$$\mathbf{k} = (\boldsymbol{k}^{(1)},\ldots,\boldsymbol{k}^{(m)})^{\mathrm{T}}, \tag{2}$$

where $\boldsymbol{k}^{(j)} = [\underline{k}_j; \overline{k}_j]$ – interval estimates with dispersion within some percent of rather known average value, $j = \overline{1,m}$ $\underline{k}_j$ – the lower, $\overline{k}_j$ – the top interval borders. Let λ_j – value corresponding to the degree of variation of the kinetic rate constant concerning a mean value k_j. Then the borders of the interval vector components $\boldsymbol{k}^{(j)}$ can be defined as $\underline{k}_j = k_j - \lambda_j k_j$ $\overline{k}_j = k_j + \lambda_j k_j$, The decision of system (1) in the conditions of (2) can be presented in the form:

$$\mathbf{x} = (\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(n)})^{\mathrm{T}}, \tag{3}$$

where $\boldsymbol{x}^{(i)} = [\underline{x}_i; \overline{x}_i]$ $i = \overline{1,n}$,

The decision of system (1) in the conditions of (2) can be received by various numerical methods of the Cauchy problem interval solution (Aris: 2000). In (Field et al.: 1974, pp. 1877-1884) the algorithm of the combined method of the sensitivity interval analysis adapted for the solution of chemical kinetics problems is described. Its main idea is reduced to the following actions (Nickel: 2014).

To assess $\overline{x}^{(i)}$ – the upper bound of $\mathbf{x}(t)$ on *i*-th coordinate, $\overline{x}^{(i)} \geq x_i$ – we will consider the system $\widetilde{\mathrm{x}}' = f(t, \widetilde{\mathrm{x}}, \widetilde{\mathrm{k}})$ $\widetilde{\mathrm{x}} \in \widetilde{\mathbf{x}}$ $\widetilde{\mathrm{k}} \in \widetilde{\mathbf{k}}$ $\widetilde{\mathrm{x}}(0) = \widetilde{\mathrm{x}}_0 \in \widetilde{\mathbf{x}}_{\mathbf{0}}$, in which:

$$\widetilde{\boldsymbol{k}}_{\mathrm{j}} = \begin{cases} \overline{\mathrm{k}}_{\mathrm{j}}, \text{ if } \boldsymbol{x}_{\mathrm{ij}}^{\mathrm{k}}(\mathrm{t}) \leq 0, \\ \underline{\mathrm{k}}_{\mathrm{j}}, \text{ if } \boldsymbol{x}_{\mathrm{ij}}^{\mathrm{k}}(\mathrm{t}) \geq 0, \\ \boldsymbol{k}_j, \text{ if } 0 \in \boldsymbol{x}_{\mathrm{ij}}^{\mathrm{k}}(\mathrm{t}), \end{cases} \qquad \widetilde{\boldsymbol{x}}_0 = \begin{cases} \overline{\mathrm{x}}_{0\mathrm{j}}, \text{if } \boldsymbol{x}_{\mathrm{ij}}^{0}(\mathrm{t}) \leq 0, \\ \underline{\mathrm{x}}_{0\mathrm{j}}, \text{if } \boldsymbol{x}_{\mathrm{ij}}^{0}(\mathrm{t}) \geq 0, \\ \boldsymbol{x}_0, \text{if } 0 \in \boldsymbol{x}_{\mathrm{ij}}^{0}(\mathrm{t}), \end{cases}$$

where $\boldsymbol{x}_{ij}^{k}(t)$ $\boldsymbol{x}_{ij}^{0}(t)$ and – interval expansions of $\partial x_i / \partial k_j$ $\partial x_i / \partial x_{0j}$ and respectively (Moore: 1979).

Interval functions $\boldsymbol{x}_{ij}^{k}(t)$ $\boldsymbol{x}_{ij}^{0}(t)$ can be defined, at the same time-solving system (1) and systems:

$$x_{ij}^{k'} = \sum_{l=1}^{n} \frac{\partial f_i}{\partial x_l}(t, \mathrm{x}, \mathrm{k}) x_{lj}^{k} + \frac{\partial f_i}{\partial x_{k_j}}(t, \mathrm{x}, \mathrm{k}), \tag{4}$$

$$x_{ij}^{k}(0)=0, i=1,...,n \;\; j=1,...,m,,$$

$$x_{ij}^{0'}=\sum_{l=1}^{n}\frac{\partial f_i}{\partial x_{x_l}}(t,\mathrm{x},\mathrm{k})x_{lj}^{0}, \qquad (5)$$

$$x_{ij}^{0}(0)=\delta_{ij}, i=1,...,n, j=1,...,n,$$

where δ_{ij} - Kronecker's symbol.

The research of the direct kinetic problem sensitivity to the variation of the kinetic parameters in some areas of uncertainty (2) consists of an assessment of the influence of kinetic model parameters on a reaction yield (Shangareeva et al.: 2016, pp. 645-649). This suggests what of speeds constants are defining at different stages of reaction. The result of solving the direct problem with interval kinetic parameters is the bilateral solution (3). It is characterized not by one dot value of concentration in each time point of reaction course, but by the interval of all possible values (Grigoryev et al.: 2016, pp. 617-622; Mustafina: 2017, pp. 805-815). The width of the received intervals of concentration can be used for an assessment of extent of rate constants influence to the corresponding concentration (Epstein et al: 1983, pp. 112-123; Mohammadi & Yekta: 2018, pp. 1-7). The widest calculated interval testifies to the greatest influence of a constant on this concentration. The narrowest interval corresponds to the smallest constant influence. To adequately assess the sensitivity of the direct problem solution the condition $\lambda_1=\lambda_2=...=\lambda_m=\lambda=const$ has to be satisfied.

In (Field et al.: 1974, pp. 1877-1884) the next way of estimation of concentration sensitivity to the various constants changes in various timepoints is offered. The result of the direct kinetic problem: (1) under the conditions (2), the solution of (4)-(5) are obtained. Then for a sensitivity assessment, it is possible to use the rated criterion, allowing to assess the constant $k_j \;\; j=\overline{1,m}$, influence on the concentration x_i $i=\overline{1,n}$, in the timepoint *t*:

$$\hat{s}_i^j = \int_{t-h}^{t} \mathrm{wid}\boldsymbol{I}(t)dt, \qquad (6)$$

$$\boldsymbol{I}(t)=\frac{\boldsymbol{k}_j \boldsymbol{x}_{ij}^{k}(t)}{\boldsymbol{x}_{\max}(t)}, \qquad (7)$$

where $\boldsymbol{x}_{ij}^{k}(t)$ – decisions of system (4) $\boldsymbol{x}_{\max}(t) = \boldsymbol{x}_{qj}^{k}(t)$ $q : \mathrm{wid}\boldsymbol{x}_{qj}^{k}(t) = \max\{\mathrm{wid}\boldsymbol{x}_{1j}^{k}(t),\ldots,\mathrm{wid}\boldsymbol{x}_{nj}^{k}(t)\}$, h – the step of a numerical method of the interval solution of Cauchy problem for the differential equations system..

3. RESULTS

The computational experiment was carried out for the reactions proceeding without the change of reaction volume (reaction of reception of phthalic anhydride) and taking into account its change (reaction of oligomerization of α-methyl styrene). We will carry out the sensitivity analysis on the example of the reaction of receiving phthalic anhydride proceeding, without the change of reaction volume (Ostrovsky et al: 1994, pp. 755-767; Laureano et al.: 2018, pp. 4-7). It should be noted that the technique given here applies to the reactions proceeding with the change of reaction environment mole number (Slinko: 2004, p. 488). We will enter the following designations: A_1 – naphthalene (initial substance), A_2 – naphthoquinone, A_3 – target product – phthalic anhydride, A_4 – carbon dioxide, A_5 – maleic anhydride. A set of the chemical transformations describing the reaction taking into account the entered designations is represented the following scheme of stages:

$$\begin{array}{lll} A_1 \to A_2, & A_2 \to A_4, & A_1 \to A_3, \\ A_1 \to A_4, & A_2 \to A_3, & A_3 \to A_5. \end{array} \qquad (9)$$

We will construct a mathematical model of considered reaction course according to the general theory of creation of the mathematical description of chemical processes (Spivak: 2009, pp. 1056-1059). According to the law of the operating masses, the kinetic equations corresponding to the (9) can be expressed the equations:

$$\begin{array}{lll} \omega_1 = k_1 x_1, & \omega_2 = k_2 x_2, & \omega_3 = k_3 x_1, \\ \omega_4 = k_4 x_1, & \omega_5 = k_5 x_2, & \omega_6 = k_6 x_3. \end{array} \qquad (10)$$

where ω_j – the j-th stage speed, $j = \overline{1,6}$, x_i – concentration of the i-th component, $i = \overline{1,5}$ k_j – the j-th reaction speed constant (s-1), $j = \overline{1,6}$. The matrix of stoichiometric coefficients is represented in table 1.

	ω_1	ω_2	ω_3	ω_4	ω_5	ω_6
x_1	-1	0	-1	-1	0	0
x_2	1	-1	0	0	-1	0

x_3	0	0	1	0	1	-1
x_4	0	1	0	1	0	0
x_5	0	0	0	0	0	1
sum	0	0	0	0	0	0

Table 1. The matrix of stoichiometric coefficients for the reaction of receiving phthalic anhydride

The reaction proceeds without a change in reaction volume, as evidenced by the last row of the matrix. Then the differential equation system describing the reaction kinetics is of the form:

$$\frac{dx_i}{dt} = f_i(t, \mathrm{x}, \mathrm{k}), t \in [0;0.6]$$
$$x_i(0) = x_i^0 \; i = \overline{1,5}, \qquad (11)$$
,.

The right parts of the equations in system (11) taking into account (10) and the matrix of stoichiometric coefficients:

$$f_1(t, \mathrm{x}, \mathrm{k}) = -\omega_1 - \omega_3 - \omega_4 = -k_1 x_1 - k_3 x_1 - k_4 x_1,$$
$$f_2(t, \mathrm{x}, \mathrm{k}) = \omega_1 - \omega_2 - \omega_5 = k_1 x_1 - k_2 x_2 - k_5 x_2,$$
$$f_3(t, \mathrm{x}, \mathrm{k}) = \omega_3 + \omega_5 - \omega_6 = k_3 x_1 + k_5 x_2 - k_6 x_3,$$
$$f_4(t, \mathrm{x}, \mathrm{k}) = \omega_2 + \omega_4 = k_2 x_2 + k_4 x_1,$$
$$f_5(t, \mathrm{x}, \mathrm{k}) = \omega_6 = k_6 x_3.$$

We will understand representation of speeds constants in the form:

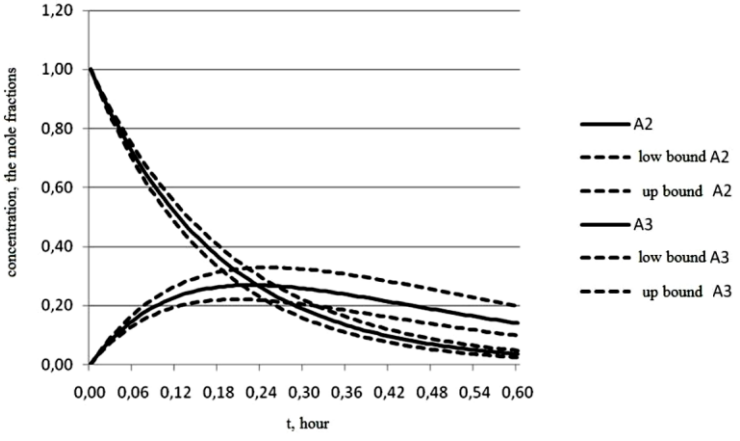
$$\boldsymbol{k}_1 = [3.19324; \; 3.3907(\qquad \boldsymbol{k}_2 = [0.61789; \; 0.65611]$$
,
$$\boldsymbol{k}_3 = [1.78577; \; 1.89623] \qquad \boldsymbol{k}_4 = [0.48209; \; 0.51191] \qquad (12)$$
,
$$\boldsymbol{k}_5 = [2.71309; \; 2.88091] \qquad \boldsymbol{k}_6 = [0.03589; \; 0.03811]$$
,

As the uncertainty of kinetic data. They form an interval vector of parameters $\mathbf{k} = (\boldsymbol{k}_1, \ldots, \boldsymbol{k}_m)$. As such, the rate constants are interval estimates with a range within 3% of the mean values calculated by the Arrhenius formula at a temperature T = 620 K, in accordance with the literature data (Tsareva: 1986;

Kalogeropoulos et al.: 2020; Nooradi et al.: 2017, pp. 71-75): $k_1 = 3.292$, $k_2 = 0.637$, $k_3 = 1.847$, $k_4 = 0.497$, $k_5 = 2.797$, $k_6 = 0.037$, forming a point parameter vector $\mathrm{k} = (k_1,\ldots,k_6)$.

Before constructing a bilateral solution of (11) under the conditions (12) we take as the initial concentration of substances degenerate intervals: $\boldsymbol{x}_1(0) = [1;1]$, $\boldsymbol{x}_i(0) = [0;0]\ i = \overline{2,5}$.

The graphic bilateral solution of the direct problem (on a target substance) for the reaction of receiving phthalic anhydride is shown in Pic. 1. In this case, the kinetic curves of changes in the concentration of substances which may be obtained by solving the direct problem with $x_1 = 1\ x_i = 0,,\ i = \overline{2,5}$ and $\forall \mathrm{k} \in \mathbf{k}$, will belong to the set of solutions, indicate the boundaries of the two-state solution.

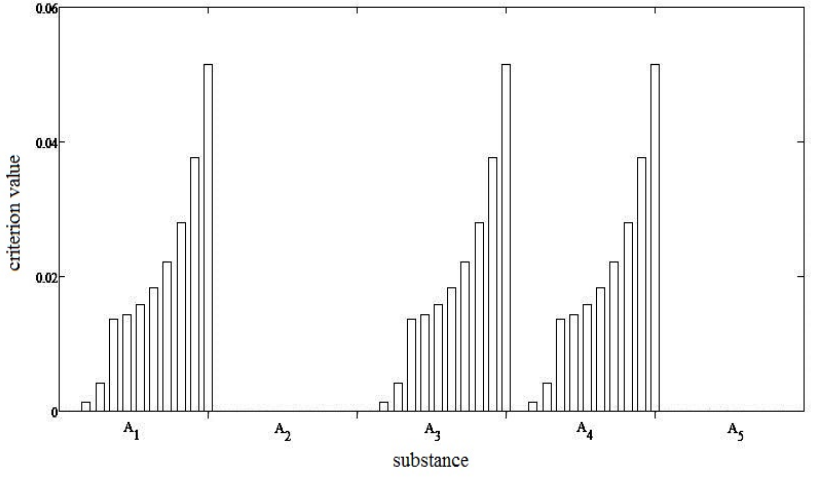


Pic. 1. Changing the concentration of naphthalene and naphthoquinone

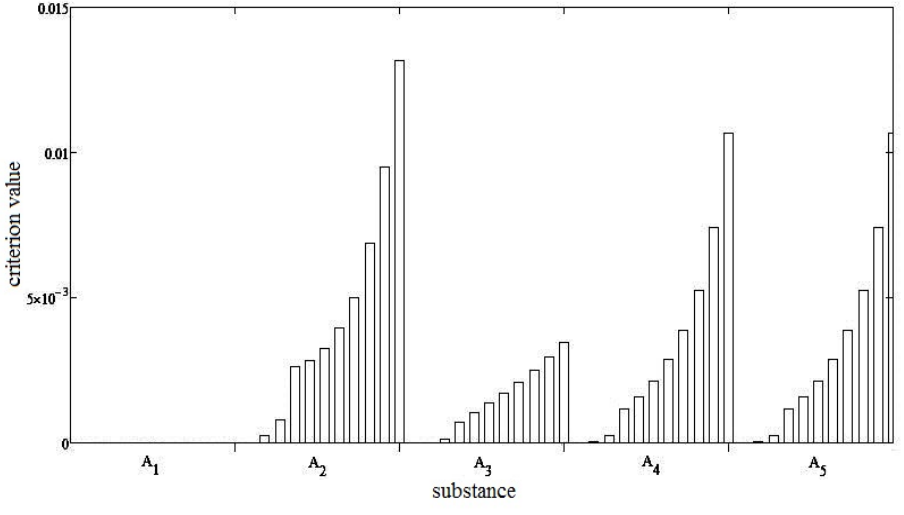
Also in this study, we analyzed the influence of variation in values of constant reaction concentrations preparation of phthalic anhydride. The analysis shows that the concentration of the reaction products A_2, A_5 are insensitive to changes in the parameter k_1, thus influence its change in limits of the considered uncertainty interval on the concentration of substances A_1, A_3, A_4 occurs practically equally. The greatest influence of the rate constant k_2 is happening about changes in the concentration of substance A_2, and only one of the five substances A_1 is independent of its variation. The rate constant k_3 does not affect the concentration A_2 but retains influence on the dynamics of the remaining reagents. The rate constant k_4 is the only parameter whose change does not remain traceless at reaction course, though the extent of its influence on concentration is rather small. The rate constant k_5 makes the maximum impact on substance A_2, not affecting the output A_4, A_5. The rate of constant k_6 has the least impact on the course of the reaction. Change of concentration of a target product depends on the degree of variation of all constants at the same time, thus, as expected, the rate constants k_1, k_2 and k_4 have the greatest impact.

Pic. 2-3 allows analyzing the substances concentration changes sensitivity in the variation of kinetic constants at certain time intervals (the number of columns in the chart, corresponding substance A_i

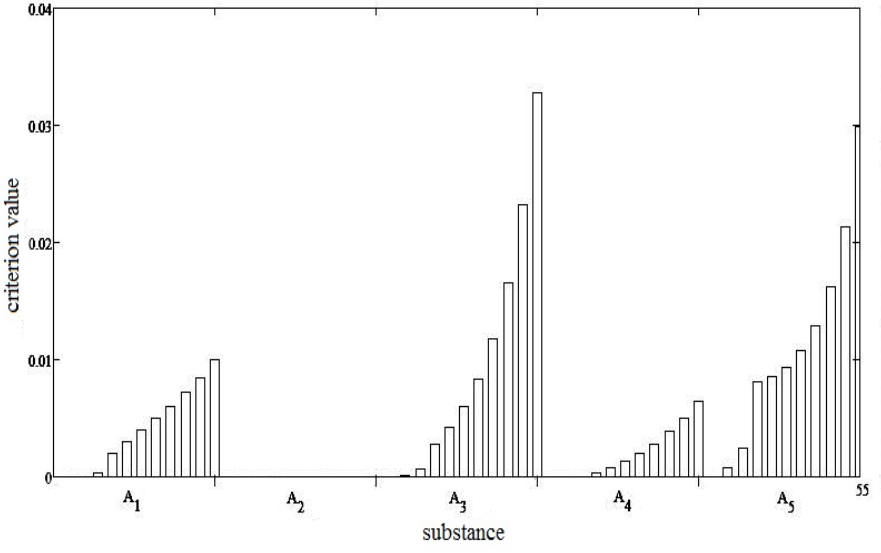
$i = \overline{1,5}$, equal to the number of segments of the partition slot in the numerical solution of the direct problem. The figures show that in all cases where the rate constant influence on the substance concentration occurs, there is a tendency to increase the width of the two-state solution of the direct problem in time. This once again confirms the Moore effect during the interval calculations.



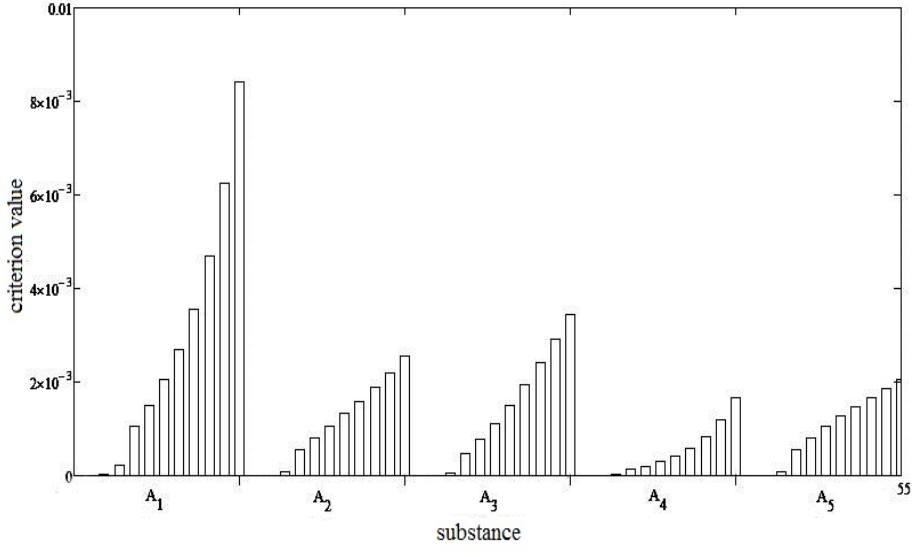
Pic. 2. The sensitivity of reagent and product concentrations of phthalic anhydride to kinetic parameters k_1.



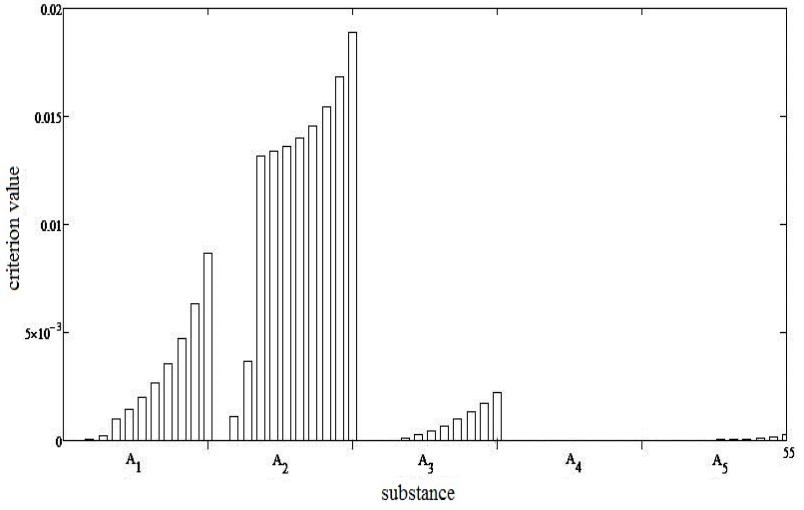
Pic. 3. The sensitivity of reagent and product concentrations of phthalic anhydride to kinetic parameters k_2.



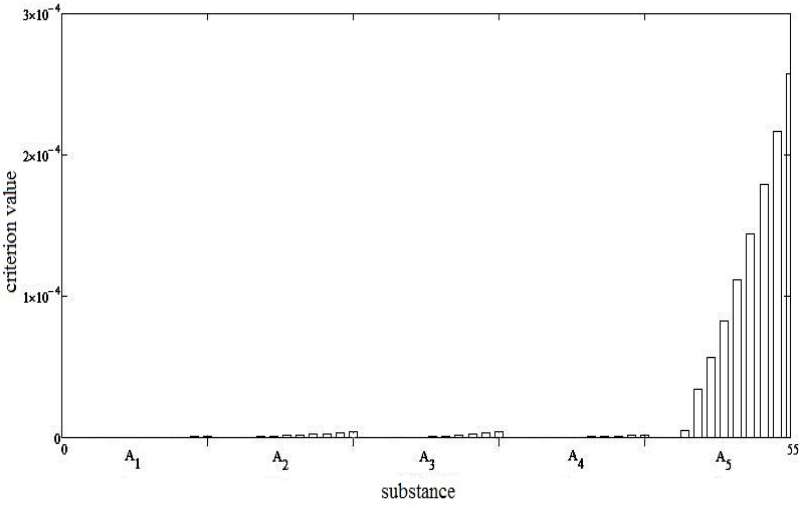
Pic. 4. The sensitivity of reagent and product concentrations of phthalic anhydride to kinetic parameters k_3.



Pic. 5. The sensitivity of reagent and product concentrations of phthalic anhydride to kinetic parameters k_4.



Pic. 6. The sensitivity of reagent and product concentrations of phthalic anhydride to kinetic parameters k_5.



Pic. 7. The sensitivity of reagent and product concentrations of phthalic anhydride to kinetic parameters k_6.

The rate constant k_4 is the only parameter whose change does not remain traceless at reaction course, though the extent of its influence on concentration is rather small. The rate constant k_5 makes the maximum impact on substance A_2, not affecting the output A_4 A_5,. The rate constant k_6 has the least impact on the course of the reaction. Change of concentration of a target product depends on the degree of variation

of all constants at the same time, thus, as expected, the rate constants k_1, k_2 k_4 and have the greatest impact.

Analyzing the results obtained by changing the porosity of the kinetic parameters in the range from 5% to 10%, we can assume that the variation of the kinetic data is not the crew dynamics grid, while the output of the main products is sensitive to porosity on average by no more than 16% -33% – for the first, 15% -30% - for the second reaction. Also, increasing the error in the kinetic parameters reduces the time interval at which it is possible to build the optimal boundaries of the set of solutions of the direct problem by the method of interval sensitivity analysis.

4. CONCLUSIONS

Thus, based on the interval analysis methods the boundaries of the chemical kinetics direct problem solution were obtained. The result analysis gained under the accuracy measurement of kinetic parameters in the range of 5% to 10% lets us conclude that kinetic data variations do not influence the dynamics of the curves, while the basic product yield is sensitive to the accuracy of not more than 15%-30% in average. Besides, when increasing the accuracy in kinetic parameters the time interval decreases. It allows modeling efficient boundaries of several direct problem solutions with the interval response analysis method.

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