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А.Н. Лабутин, В.Ю. Невиницын

Александр Николаевич Лабутин, Владимир Юрьевич Невиницын (✉)

Кафедра технической кибернетики и автоматики, Ивановский государственный химико-технологический университет, пр. Шереметевский, 7, Иваново, Российская Федерация, 153000

E-mail: lan@isuct.ru, nevinityn@gmail.com (✉)

**СИНТЕЗ НЕЛИНЕЙНОГО АЛГОРИТМА УПРАВЛЕНИЯ ХИМИЧЕСКИМ РЕАКТОРОМ
С ИСПОЛЬЗОВАНИЕМ СИНЕРГЕТИЧЕСКОГО ПОДХОДА**

В работе решена задача аналитического синтеза синергетической системы управления химическим реактором для реализации сложной последовательно-параллельной экзотермической реакции. Синтез законов управления осуществляется с использованием метода аналитического конструирования агрегированных регуляторов. Химический реактор является одним из основных аппаратов в химической промышленности. Несмотря на значительное количество работ, связанных с автоматизацией и управлением химическими реакторами, проблема синтеза систем управления, обеспечивающих поддержание оптимальных режимов их работы, остается до конца не решенной. Это объясняется основной особенностью химических реакторов как объектов управления: многомерностью, нелинейностью и многосвязностью. Выходом из данной ситуации является развитие физической теории управления и в частности синергетической теории управления. Использование идей синергетики в задачах управления предполагает разработку и реализацию способа направленной целевой самоорганизации диссипативных нелинейных систем “объект–регулятор”. При этом цель движения системы формулируется в виде желаемого инвариантного многообразия в фазовом пространстве объекта, выполняющего роль целевого аттрактора. В работе рассмотрен химический реактор емкостного типа, снабженный механической мешалкой и теплообменной рубашкой. Аппарат функционирует в политропическом режиме. В реакторе реализуется многостадийная последовательно-параллельная экзотермическая реакция. Целью функционирования химического реактора является получение целевого продукта заданной концентрации. Задача системы управления реактором заключается в стабилизации концентрации целевого компонента и температуры реакционной смеси в аппарате на заданных значениях в условиях действия возмущений на объект. Используя метод аналитического конструирования агрегированных регуляторов на основе параллельно–последовательной совокупности инвариантных многообразий, синтезирован нелинейный алгоритм управления, решающий задачу стабилизации концентрации целевого компонента и температуры смеси. Компьютерное моделирование

замкнутой системы “объект–регулятор” подтвердило такие свойства синтезированной системы управления, как инвариантность к возмущениям, ковариантность с задающими воздействиями и асимптотическая устойчивость. Данные обстоятельства делают синергетическую теорию управления весьма перспективной применительно к таким сложным, многосвязным и нелинейным объектам химической технологии, как химические реакторы.

Ключевые слова: аналитический синтез, система управления, химический реактор, синергетическая теория управления, компьютерное моделирование

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A.N. Labutin, V.Yu. Nevinitsyn

Alexander N. Labutin, Vladimir Yu. Nevinitsyn (✉)

Department of Technical Engineering Cybernetics and Automation, Ivanovo State University of Chemistry and Technology, Sheremetievskiy ave., 7, Ivanovo, 153000, Russia

E-mail: lan@isuct.ru, nevinitsyn@gmail.com (✉)

SYNTHESIS OF CHEMICAL REACTOR NONLINEAR CONTROL ALGORITHM USING SYNERGETIC APPROACH

The problem of analytical synthesis of synergetic control system of chemical reactor for realization of a complex series–parallel exothermal reaction has been solved. The synthesis of control principles is performed using the analytical design method of aggregated regulators. A chemical reactor is one of the common apparatuses in chemical industry. Despite a large number of the works related to automation and control of chemical reactors, the problem of synthesizing control systems that provide the maintenance of optimal modes of their operation remains practically unsolved. This is related to the principal feature of chemical reactors as controlled objects, namely, manifold, non-linearity, and multi-coupling. An outcome from this situation is to develop a physical theory of control, in particular synergetic control theory. The use of synergism ideas in the problems of control assumes the development and realization of a method of directed target self-organization of dissipative non-linear systems “object-regulator”. Furthermore, the aim of the motion of a system is formulated as the desired invariant manifold in a phase space of the object, which acts as a target attractor. The paper deals with continuous stirred tank reactor equipped with a mechanical stirrer and cooling jacket. The reactor operates in the polytropic mode. The multistep series-parallel exothermic process is carried out in the reactor. The objective of chemical reactor operation is to obtain the key product of specified concentration. The aim of chemical reactor control system is to maintain both concentration of desired product and temperature of reaction mixture in the device at the given values under the action of disturbances on the object. Using the analytical design method of aggregated regulators on the basis of parallel-series combination of invariant manifolds, a non-linear control algorithm was synthesized, which solves the problem of stabilization of the concentration of the target component and mixture temperature. Computer simulation of the object–regulator isolated system confirmed these properties of synthesized control system as the disturbance invariance, covariance to the given actions, and asymptotic stability. These facts make synergetic control theory very promising for application for such complex, manifold, and nonlinear objects of chemical engineering as chemical reactors.

Key words: analytical synthesis, controlled system, chemical reactor, synergetic control theory, computer simulation

INTRODUCTION

During the step of the design of chemical production, which is related to the conversion of initial substances to final products, the problem of optimal synthesis of a reactor unit and problem of synthesis of the process control algorithms should be solved; and, at the step of industrial operation, the sub-problem of organization of optimal functioning of the object under the effect of parametrical and signal disturbances must be solved too [1-5].

Despite the large number of the works related to the automation and control of chemical reactors [6-9], the problem of control systems synthesis that provide the maintenance of optimal modes of their work remains practically unsolved. This can be explained by the principal features of chemical reactors as controlled objects, namely, manifold, nonlinearity, and multi-coupling.

A possible outcome from this situation is to develop a physical theory of control, in particular synergetic control theory, the principal features of which were formulated in [10-12].

The use of synergism ideas in the problems of control assumes the development and realization of the directed target self-organization of "object-regulator" dissipative nonlinear systems. It is supposed that the aim of a system motion is formulated as the desired invariant manifold in the phase space of an object, which acts as a target attractor [12].

In general, the problem of synergetic synthesis of the control system is formulated as follows: the control principle, $u = (u_1, \dots, u_m)^T$ should be determined as the function of state variables of object $u_1(x_1, \dots, x_n), \dots, u_m(x_1, \dots, x_n)$, which transforms the representation point (RP) of a system in the phase space from the random initial state to the neighborhood of the given invariant manifolds $\psi_S(x_1, \dots, x_n) = 0, S = 1, \dots, m$, and subsequent motion along the intersection of the manifolds to any stationary point or to any dynamic mode. In the given relationships, n is the dimension of the state vector and m is the number of external controls. On the trajectory of the motion, the minimum of the criterion of optimality of system (J) must be reached and its stability should be ensured as follows:

$$J = \int_0^{\infty} \left[\sum_{S=1}^m \left(T_S^2 \dot{\psi}_S^2 + \psi_S^2 \right) \right] d\tau. \quad (1)$$

The motion of RP in the phase space follows the functional equation

$$T_S \dot{\psi}_S + \psi_S = 0, \quad S = 1, \dots, m, \quad (2)$$

where T_S is the time constant. This is the equation of the stable extremal, which gives minimum to the ob-

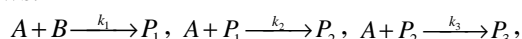
jective functional (1). The condition of asymptotic stability of the entire system generally has the form $T_S > 0$.

The efficiency of the method of analytical design of control algorithms for nonlinear objects by means of synergetic principle (the method of analytical design of aggregated regulators (ADAR)) is shown in [13-16].

In this work, the problem of synthesis the effective control algorithms for the chemical reactor in the realization of the complex series-parallel reaction is stated. The synthesized control system should provide stabilization of the concentration of the target component of a chemical reaction in the apparatus out-flow and mixture temperature in the apparatus under the action of disturbances on object.

OBJECT DESCRIPTION AND STATEMENT OF CONTROL PROBLEM

A chemical reactor is a volume-type apparatus equipped with a mechanical stirrer and cooling jacket (Fig. 1). It is functioning in the polytropic mode. The multistep series-parallel exothermic reaction of oxy-ethylation of butyl alcohol is occurs in the reactor as follows:



where A and B are the initial reagents; P_1, P_2 , and P_3 are the products of the reaction; k_1, k_2 , and k_3 are the rate constants of the stages. The key component is P_2 substance. The initial reagents A and B are fed to the device by separate flows.

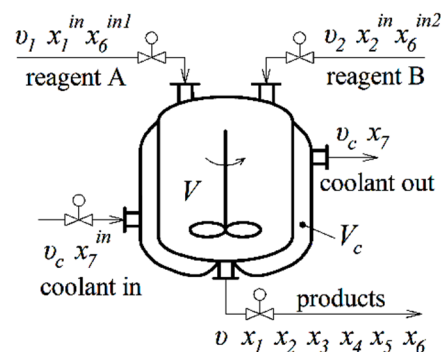


Fig. 1. The schematic diagram of chemical reactor
Рис. 1. Принципиальная схема химического реактора

In Fig. 1, the following nomenclature is used: x_1^in, x_2^in are the concentrations of initial reagents; v_1, v_2 are the flow rates of initial reagents; x_6^in1, x_6^in2 are the temperatures of initial reagents; x_7^in, x_7 are the coolant temperatures at the inlet and outlet of reactor; v_c is the coolant flow rate at the inlet and outlet of reactor; x_6 is the temperature of reaction mixture in the apparatus; v is the use of reaction mixture on the exit from device;

x_1, x_2, x_3, x_4 , and x_5 are the concentrations of components A, B, P_1, P_2 , and P_3 in reactor; V is the volume of reaction mixture in the operating volume; and V_c is the volume of coolant in jacket.

The objective of chemical reactor operation is to obtain the key component of specified concentration. Therefore, the aim of chemical reactor control system is to maintain both concentration of desired product and temperature of reaction mixture at the given set points (values) under the action of disturbances, i.e. $x_4 = \bar{x}_4, x_6 = \bar{x}_6$ where \bar{x}_4 and \bar{x}_6 are the given values of concentration and temperature, respectively. The flow rate of the initial reagent v_2 and the coolant flow rate v_c at the input to the device are chosen as the control parameters for concentration and temperature regulation, respectively.

The mathematical model of chemical reactor has the following form:

$$\begin{aligned} \frac{dx_1}{d\tau} &= R_1 + M_A - b_2x_1 - b_3x_1u_1 \\ \frac{dx_2}{d\tau} &= R_2 - b_2x_2 + (M_B - b_3x_2)u_1 \\ \frac{dx_3}{d\tau} &= R_3 - b_2x_3 - b_3x_3u_1 \\ \frac{dx_4}{d\tau} &= R_4 - b_2x_4 - b_3x_4u_1 \\ \frac{dx_5}{d\tau} &= R_5 - b_2x_5 - b_3x_5u_1 \\ \frac{dx_6}{d\tau} &= \alpha_1k_1x_1x_2 + \alpha_2k_2x_1x_3 + \alpha_3k_3x_1x_4 + b_2x_6^{in1} + \\ &+ \beta_1x_7 - (\beta_1 + b_2)x_6 + (x_6^{in2} - x_6)b_3u_1 \\ \frac{dx_7}{d\tau} &= \beta_2(x_6 - x_7) + b_1(x_7^{in} - x_7)u_2 \end{aligned} \quad (3)$$

where $R_1 = -k_1x_1x_2 - k_2x_1x_3 - k_3x_1x_4, R_2 = -k_1x_1x_2, R_3 = k_1x_1x_2 - k_2x_1x_3, R_4 = k_2x_1x_3 - k_3x_1x_4, R_5 = k_3x_1x_4$ is the rate of reaction for components; $M_A = v_1x_1^{in} / V; M_B = x_2^{in} / V; b_1 = 1/V_c; b_2 = v_1 / V; b_3 = 1/V; \alpha_i = \Delta H_i / (\rho C), i = 1, \dots, 3; \beta_1 = K_T F_T / (\rho C V); \beta_2 = K_T F_T / (\rho C C V_c); \Delta H_i, i = 1, \dots, 3$ is the heat of reaction for its corresponding stage; ρ, C are the density and heat capacity of reaction mixture; ρ_c, C_c are the density and heat capacity of coolant; K_T is the heat transfer coefficient; F_T is the heat transfer surface; $k_i = k_{i0} \cdot \exp(-E_i / R(x_6 + 273)), i = 1, \dots, 3$ is the reaction rate constant; $k_{i0}, i = 1, \dots, 3$ is the pre-exponential multiplier of rate constant; $E_i, i = 1, \dots, 3$ is the activation energy; R is the gas constant; and $u_1 = v_2, u_2 = v_c$ are the control parameters.

The analysis of structure of the set of equations of mathematical model of reactor (3) shows that control parameter u_1 acts on variable x_4 directly. The control parameter u_2 acts on the variable x_6 indirectly through the variable x_7 . Thus, the control channels for the concentration and temperature of reaction mixture in the apparatus can be represented as follows: $u_1 \rightarrow x_4, u_2 \rightarrow x_7 \rightarrow x_6$.

SYNTHESIS OF CONTROL PRINCIPLES BY MEANS OF ADAR METHOD

Because the mathematical model of the object (3) contains two external control parameters $u_1 = v_2$ and $u_2 = v_c$, we use the ADAR method on the basis of parallel-series combination of invariant manifolds [12]. The procedure for synthesis the control principle consists of the following steps. At the first step, the invariant manifolds are considered as shown below:

$$\psi_S(x_1, \dots, x_7) = 0, S = 1, 2,$$

which determines the given relationships between phase coordinates of object, which, in turn, reflects the features of the controlled object and requirements of a designer to the system. The control principle $u = (u_1, u_2)^T$ is synthesized so as to perform the transition of the representation point of system in phase space from arbitrary initial position to the intersection of manifolds, $\psi_{1,2}(x_1, \dots, x_7) = 0$.

Let us introduce two aggregated macro-variables, the first of which reflects the technological requirement to the concentration of target component and the second determines the relationship of x_7 with controlled variable x_6 as follows:

$$\psi_1 = x_4 - \bar{x}_4, \psi_2 = x_7 + v_1(x_6), \quad (4)$$

where $v_1(x_6)$ is somewhat function, which should be determined at subsequent procedure of synthesis. Macro-variables (4) should follow the solution of principal functional equation of ADAR method (2).

Let us substitute the macro-variables ψ_1 and ψ_2 of Eq. (4) to the functional equation (2) for the synthesis of control principle $u = (u_1, u_2)^T$. As the result, we obtain the following equations:

$$\begin{aligned} T_1 \frac{dx_4}{d\tau} + x_4 - \bar{x}_4 &= 0 \\ T_2 \left[\frac{dx_7}{d\tau} + \frac{\partial v_1}{\partial x_6} \cdot \frac{dx_6}{d\tau} \right] + x_7 + v_1 &= 0 \end{aligned}$$

Due to the equations of the object (3) these relationships become:

$$\begin{aligned} T_1 (R_4 - b_2x_4 - b_3x_4u_1) + x_4 - \bar{x}_4 &= 0 \\ T_2 \left[\beta_2(x_6 - x_7) + b_1(x_7^{in} - x_7)u_2 + \frac{\partial v_1}{\partial x_6} \cdot (f_6 + \right. & \quad (5) \\ \left. + \beta_1x_7 + (x_6^{in2} - x_6)b_3u_1) \right] + x_7 + v_1 &= 0 \end{aligned}$$

where $f_6 = \alpha_1 k_1 x_1 x_2 + \alpha_2 k_2 x_1 x_3 + \alpha_3 k_3 x_1 x_4 + b_2 x_6^{in1} - (\beta_1 + b_2) x_6$.

The following relationships for the control principle follow from Eq. (5):

$$\begin{aligned} u_1 &= \frac{(x_4 - \bar{x}_4)}{T_1 b_3 x_4} + \frac{R_4}{b_3 x_4} - \frac{b_2}{b_3} \\ u_2 &= -\frac{(x_7 + v_1)}{T_2 b_1 (x_7^{in} - x_7)} - \frac{\beta_2 (x_6 - x_7)}{b_1 (x_7^{in} - x_7)} - \\ & - \frac{\partial v_1}{\partial x_6} \cdot \frac{[f_6 + \beta_1 x_7 + (x_6^{in2} - x_6) b_3 u_1]}{b_1 (x_7^{in} - x_7)} \end{aligned} \quad (6)$$

Control parameters u_1 and u_2 transfer the RP of the system in the phase space to the intersection of manifolds $\psi_1 = 0$ and $\psi_2 = 0$, where the relationships $x_4 = \bar{x}_4$, $x_7 = -v_1$ are realized and “the compression of phase space” can be observed, i.e., the decrease of dimension of the set of equations (3) occurs. The equations of decomposed system, taking into account the relationship $x_7 = -v_1$, takes the following form:

$$\begin{aligned} \frac{dx_1}{d\tau} &= R_1 + M_A - b_2 x_1 - b_3 x_1 u_1 \\ \frac{dx_2}{d\tau} &= R_2 - b_2 x_2 + (M_B - b_3 x_2) u_1 \\ \frac{dx_3}{d\tau} &= R_3 - b_2 x_3 - b_3 x_3 u_1 \\ \frac{dx_5}{d\tau} &= R_5 - b_2 x_5 - b_3 x_5 u_1 \\ \frac{dx_6}{d\tau} &= f_6 - \beta_1 v_1 + (x_6^{in2} - x_6) b_3 u_1 \end{aligned} \quad (7)$$

The function $v_1(x_6)$ in the decomposed system (7) can be considered as the “internal” control, under the action of which the motion of object (7) along the intersection of manifolds $\psi_{1,2} = 0$ takes place.

At the second step of procedure, the investigation of the expression for $v_1(x_6)$ is performed. For this purpose, the aim of the motion of system (7) is considered in the form of invariant manifold, which describes the technological requirement to the system as follows:

$$\psi_3 = x_6 - \bar{x}_6 = 0 \quad (8)$$

Macro-variable ψ_3 meets the solution to the functional equation $T_3 \dot{\psi}_3 + \psi_3 = 0$. Taking into account the relationship (8) and the model of decomposed system (7), it can be written as follows:

$$T_3 (f_6 - \beta_1 v_1 + (x_6^{in2} - x_6) b_3 u_1) + x_6 - \bar{x}_6 = 0. \quad (9)$$

“The internal control” due to Eq. (9) can be written as:

$$v_1 = \frac{(x_6 - \bar{x}_6)}{T_3 \beta_1} + \frac{f_6}{\beta_1} + \frac{(x_6^{in2} - x_6) b_3 u_1}{\beta_1}. \quad (10)$$

Final expression for the control principle $u = (u_1, u_2)^T$ can be obtained by substitution of the function v_1 (10) and its partial derivative $\partial v_1 / \partial x_6$ to Eq. (6). The parameters of the control law adjustment, which affect the quality of the dynamics of the processes in object-regulator isolated system, are the time constants T_1 , T_2 and T_3 . The conditions of asymptotic stability have the following form: $T_1 > 0$, $T_2 > 0$, $T_3 > 0$.

RESULTS AND DISCUSSION

In order to verify the workability of the synthesized control law for the chemical reactor, the computer simulation of the object-regulator closed system was performed. Properties of the control system, such as the disturbance invariance, covariance to the given disturbance, and the asymptotic stability of closed system were also studied.

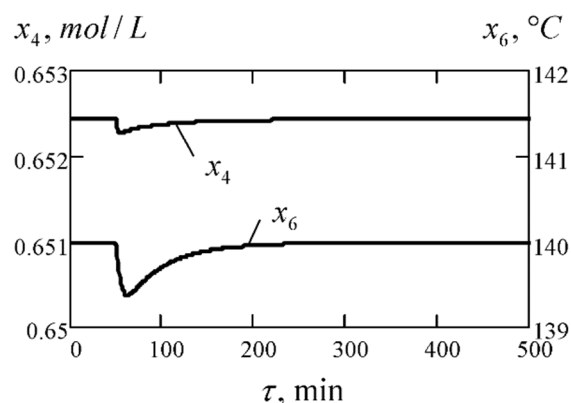


Fig. 2. The change in controlled variables after the inflow v_1 decrease (10%)

Рис. 2. Изменение регулируемых переменных при уменьшении расхода v_1 на 10%

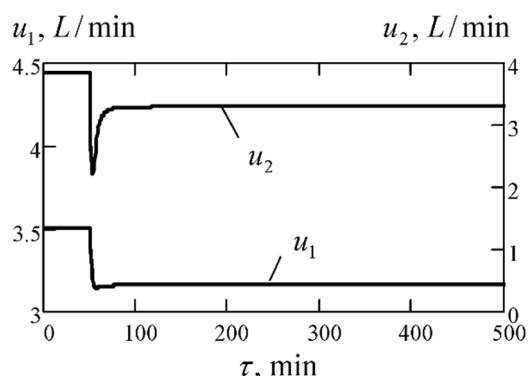


Fig. 3. The change in control actions after the inflow v_1 decrease (10%)

Рис. 3. Изменение управляющих воздействий при уменьшении расхода v_1 на 10%

The simulation was performed with the following technological and design parameters of the object: $V = 500$ L, $V_c = 290$ L, $x_1^{in} = 19.74$ mol/L, $x_2^{in} = 10.93$ mol/L, $v_1 = 1.5$ L/min, $v_2 = 3.5$ L/min, $v = 5.0$ L/min, $v_c = 3.84$ L/min, $x_6^{in} = 20$ °C, $x_6^{in2} = 30$ °C, $x_7^{in} = 20$ °C,

$K_T = 12 \text{ kJ}/(\text{m}^2 \text{ min K})$, $F_T = 2.9 \text{ m}^2$, $\rho = 0.9 \text{ kg/L}$, $C = 2 \text{ kJ}/(\text{kg K})$, $\rho_c = 1 \text{ kg/L}$, $C_c = 4.18 \text{ kJ}/(\text{kg K})$, $\Delta H_1 = \Delta H_2 = \Delta H_3 = 80 \text{ kJ/mol}$, activation energy $E_1 = 48635 \text{ J/mol}$, pre-exponential multiplier of the rate constant $k_1 k_{10} = 109860 \text{ L}/(\text{mol min})$, ratio of the rate constants for consecutive stages $k_2/k_1 = 2$, $k_3/k_1 = 2.5$, given concentration of target component $\bar{x}_4 = 0.652 \text{ mol/L}$, and the given temperature of reaction mixture $\bar{x}_6 = 140^\circ\text{C}$. The parameters of adjustment of regulators are $T_1 = 50 \text{ min}$, $T_2 = 15 \text{ min}$, and $T_3 = 15 \text{ min}$.

In Figs. 2, 3, the examples of transient controlled processes in the object–regulator in the system are shown. The simulation results presented here deal with the effect of step disturbance with change inflow v_1 . At the initial time the chemical reactor operates in static mode. There is a step increase inflow v_1 at the time point $\tau = 50 \text{ min}$. From this time the control parameters $u_1 = v_2$ and $u_2 = v_c$ are computed according to Eq. (6). Then there are concentration and temperature control processes are in progress. In the course of time the controlled variables x_4 and x_6 take desired values. The steady-state error is zero. As follows from Figs. 2, 3, the synthesized control law of the chemical reactor ensures disturbance invariance with change inflow v_1 .

CONCLUSIONS

In this work, the problem of the analytical synthesis of the control law of chemical reactor was solved by means of the methods of synergetic theory. Synthesized nonlinear control law solves the problem of stabilization of the concentration of the target component and mixture temperature under the action of disturbances in the object. Computer simulation of the object–regulator closed system confirmed these properties of synthesized control system as the disturbance invariance, covariance to the given actions (set points), and

asymptotic stability. These facts make synergetic control theory very promising for application to such complex, manifold, and nonlinear objects of chemical engineering as chemical reactors.

NOMENCLATURE

V – volume of reaction mixture in device, L;
 V_c – volume of coolant in jacket, L;
 v_1, v_2 – consumption of initial reagents on the enter to device, L/min;
 v – consumption of reaction mixture on the exit from reactor, L/min;
 v_c – coolant flow rate at the inlet and outlet of reactor, L/min;
 k_1, k_2 , and k_3 – rate constants of steps, L/(mol min);
 k_{10} – preexponential multiplier of rate constant k_1 , L/(mol min);
 R_1, R_2, R_3 , and R_4 – rate constant on components, mol/(L min);
 u_1, u_2 – controlling actions, L/min;
 $x_1^{\text{in}}, x_2^{\text{in}}$ – concentrations of initial reagents, mol/L;
 $x_6^{\text{in}1}, x_6^{\text{in}2}$ – temperatures of initial reagents, $^\circ\text{C}$;
 x_7^{in} – coolant temperature at the inlet of reactor, $^\circ\text{C}$;
 x_1, x_2, x_3, x_4 , and x_5 – concentrations of components A, B, P₁, P₂, and P₃ in reactor, mol/L;
 K_T – heat transfer coefficient, $\text{kJ}/(\text{m}^2 \text{ min K})$;
 F_T – heat transfer surface, m^2 ;
 ρ, ρ_c – densities of reaction mixture and coolant, kg/L ;
 C, C_c – heat capacities of reaction mixture and coolant, $\text{kJ}/(\text{kg K})$;
 $\Delta H_1, \Delta H_2$ and ΔH_3 – heat of reaction for its corresponding stage, kJ/mol ;
 E_1, E_2 , and E_3 – activation energies, J/mol ;
 R – the gas constant, $\text{J}/(\text{mol K})$;
 \bar{x}_4 – given value of concentration of target component, mol/L;
 \bar{x}_6 – given value of temperature of reaction mixture in the apparatus, $^\circ\text{C}$;
 T_1, T_2 and T_3 – time constants, min;
 τ – time, min.

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