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SYNERGETIC CONTROL OF NONLINEAR DYNAMIC OBJECTS

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Abstract: *Considers the synthesis of effective control algorithms for a chemical reactor, which is the main one in the production of butyl alcohol. The method based on synergetic approach for transferring the apparatus from one capacity to another (specified) maintaining the required quality of the target component is proposed in order to ensure the stabilization of the concentration of target component at the outlet of the reactor under the conditions of uncertain disturbances affecting to an object. A mathematical model of the process based on a stoichiometric matrix taking into account the physicochemical properties of the process is developed. The control algorithm was synthesized by the method of analytical design of an aggregate controller that provides the necessary property of a control system for a chemical reactor. The mathematical model of the process serves as the basis for the selection of attractors of phase variables. The proposed method for synthesizing a control system based on a synergistic approach has made it possible to better stabilize the temperature regime of the process and the concentration of chemical reagents.*

Keywords: *synergistic synthesis, target component, asymptotic stability, stoichiometric matrix, method.*

Аннотация: *Бутил спиртини олишда асосий ўрин эгаллйдиган кимёвий реакторни бошқаришнинг самарали алгоритмларини синтез қилиш масалалари ёритиб берилган. Объектга наоиқ ғалаёнлар таъсир кўрсатганда реакторнинг чиқишидаги мақсадли компонентларнинг концентрациясини стабиллашни таъминлаш, шунингдек мақсадли компонентнинг сифатини сақлаб қолган ҳолда қурилманинг бир ишлаб чиқариш қувватидан бошқасига (берилганга) ўтказиш учун синергетик ёндашувга асосланган усул таклиф этилган. Жараённинг физик-кимёвий хоссаларини инобатга олган ҳолда жараённинг стехиометрик матрицасига асосланган математик модели ишлаб чиқилган. Кимёвий реакторнинг бошқариш системасини зарурий хоссаларини таъминловчи бошқариш алгоритми агрегатлаштирилган ростлагичларни аналитик лойиҳалаш усули асосида синтезланган. Жараённинг математик модели фазовий ўзгарувчилар аттракторини танлаш учун ҳизмат қилади. Таклиф қилинган синергетик ёндашув асосида бошқариш тизимини синтезлаш усули кимёвий реагентларнинг концентрациясини ҳамда жараённинг ҳарорат режимини янада сифатли барқарорлаш имконини беради.*

Калит сўзлар: *синергетик синтез, мақсадли компонент, асимптотик тургунлик, стехиометрик матрица, усул.*

Аннотация: *Рассмотрены вопросы синтеза эффективных алгоритмов управления химическим реактором, являющего основным аппаратом в получении бутилового спирта. Для обеспечения стабилизации концентрации целевого компонента на выходе из реактора в условиях действия на объект неопределенных возмущений, а также перевода аппарата с одной производительности на другую (заданную) с сохранением требуемого качества целевого компонента предложен метод, основанный на синергетическом подходе. Разработана математическая модель процесса на основе стехиометрической матрицы с учетом физико-химических свойств процесса. Синтез алгоритма управления осуществлялся методом аналитического конструирования агрегированного регулятора, обеспечивающего необходимое свойство системы управления химическим реактором. Математическая модель процесса служила основой для выбора аттракторов фазовых переменных. Предложенный способ синтеза системы управления на основе синергетического подхода позволил более качественно стабилизировать температурный режим процесса и концентрации химических реагентов.*

Ключевые слова: *синергетический синтез, целевой компонент, асимптотическая устойчивость, стехиометрическая матрица, метод.*

Introduction

One of the main apparatuses of food industry enterprises in the technological scheme for producing butyl alcohol is a chemical reactor, the purpose of which is to ensure at its output a predetermined optimal concentration value provided for in the technological regulations of the target product. It is known that a chemical reactor is an energy-consuming object. In this regard, the economic efficiency of the entire production largely depends on ensuring the normal functioning of the chemical reactor and its performance. The main feature of chemical reactors as control objects is their multidimensionality, as well as the uncertainty of the concentration of the initial mixture. Currently, there are a sufficient number of publications related to the automation and control of chemical reactors, the problem of the synthesis of control systems that ensure the maintenance of optimal operating conditions, which has not been solved, is related to the complexity of the processes occurring in the reactors. Modern complex systems of diverse nature constitute a complex of various subsystems that perform certain technological functions and are interconnected by processes of intense dynamic interaction and energy exchange of matter and information. The indicated super systems are nonlinear, multidimensional, and multiply connected, in which complex transient processes occur and critical and chaotic regimes arise. The control problems of such dynamic systems are very relevant, difficult and practically inaccessible to the existing control theory [1].

A huge number of various chemical processes are implemented in the chemical industry and related industries, differing in the type of chemical reaction, thermodynamic parameters, kinetic characteristics (conversion scheme, kinetic model), phase composition of the starting reagents and reaction mixture, as well as the design and type of reactors [2]. In many cases, the reactor subsystem is central in the general scheme for converting the starting reagents into target products and to a large extent determines the resources and energy saving, the economic efficiency of the production process as a whole, and the degree of satisfaction of consumer demand for certain products. In the class of linear systems, to ensure robustness, adaptive automatic control systems with parameter adjustment, inertialess state controllers, robust systems based on typical PID controllers, and fuzzy control systems are used. However, these approaches are ineffective in the synthesis of control systems for essentially nonlinear objects. The ADAR method, developed in the framework of the synergetic theory of control, seems to be promising in this regard [3]. Synergetic methods based on nonlinear dynamics and nonequilibrium thermodynamics allow both successful research of various chemical-technological processes and efficient control of them [4].

Research Methods and the Received Results

A chemical reactor is a continuous capacitive apparatus operating in the polytropic mode (Fig.1). As a model reaction, a liquid-phase series-parallel reaction of butyl alcohol hydroxyethylation was chosen, which is of great practical importance [5]. The stoichiometric reaction equations have the form:

$$\begin{aligned} &CH_2-CH_2 + C_4H_9OH \xrightarrow{k_1} C_4H_9OC_2H_4OH \\ &\quad\ \ O \\ &C_4H_9OC_2H_4OH + CH_2-CH_2 \xrightarrow{k_2} C_4H_9O(C_2H_4O)_2H \\ &\qquad\qquad\quad\ \ O \\ &C_4H_9O(C_2H_4O)_2H + CH_2-CH_2 \xrightarrow{k_3} C_4H_9O(C_2H_4O)_3H \\ &\qquad\qquad\qquad\ \ O \end{aligned} \qquad (1)$$

For the mathematical formalization of the process, we introduce the following notation:

$$A-CH_2-CH_2$$
$$\quad\ \ O$$

$$\begin{aligned} B &- C_4H_9OH; \\ C_1 &- C_4H_9OC_2H_4OH; \\ C_2 &- C_4H_9O(C_2H_4O)_2H; \\ C_3 &- C_4H_9O(C_2H_4O)_3H; \end{aligned} \quad (2)$$

Taking into account the notation (2), chemical reactions (1) will take the following form:

$$\begin{aligned} A+B &\to C_1 \\ A+C_1 &\to C_2 \\ A+C_2 &\to C_3 \end{aligned} \quad (3)$$

Matrix of stoichiometric coefficients $\nu_{ij}, i=\overline{1,9}, j=\overline{1,4}$, The corresponding kinetic equations are presented in Table 1.

Table 1.

Matrix of stoichiometric coefficients

	CH_2-CH_2 (O)	C_4H_9OH	$C_4H_9OC_2H_4OH$	$C_4H_9O(C_2H_4O)_2H$	$C_4H_9O(C_2H_4O)_3H$
ω_1	-1	-1	-1	0	0
ω_2	-1	0	-1	1	0
ω_3	-1	0	0	-1	0

The resulting matrix is a matrix of stoichiometric coefficients, which formally represents the rate of change of the components of a chemical reaction. According to the law of the acting masses and the matrix of stoichiometric coefficients (Tab.1), the kinetic equations corresponding to the chemical transformation scheme (3) for the process can be expressed by the equations

$$\begin{aligned} \omega_1 &= k_1 Cx_1 Cx_2; \\ \omega_2 &= k_2 Cx_3 Cx_1; \\ \omega_3 &= k_3 Cx_4 Cx_1; \end{aligned} \quad (4)$$

where, C_{xi} – vector of molar concentrations of substances, mol/m^3; $k_1 - k_2 -$ rate constants (sec^{-1}) chemical reactions of the corresponding direction.

The rate of change of each x_i – component has the following form [6]:

$$\begin{aligned} g_{x_1} &= -\omega_1 - \omega_2 - \omega_3; \\ g_{x_2} &= \omega_1; \\ g_{x_3} &= \omega_1 - \omega_2; \\ g_{x_4} &= \omega_2 - \omega_3; \\ g_{x_5} &= \omega_3; \end{aligned} \quad (5)$$

The kinetics of the reaction is described by a system of equations

$$\begin{cases} \frac{dx_1}{dt} = -k_1 \cdot x_1 \cdot x_2 - k_2 \cdot x_1 \cdot x_3 - k_3 \cdot x_1 \cdot x_4 \\ \frac{dx_2}{dt} = -k_1 \cdot x_1 \cdot x_2 \\ \frac{dx_3}{dt} = k_1 \cdot x_1 \cdot x_2 - k_2 \cdot x_1 \cdot x_3 \\ \frac{dx_4}{dt} = k_2 \cdot x_1 \cdot x_3 - k_3 \cdot x_1 \cdot x_4 \\ \frac{dx_5}{dt} = k_3 \cdot x_1 \cdot x_4 \end{cases} \quad (6)$$

where x_1, x_2 - are the concentrations of reagents *A* and *B;* x_3, x_4, x_5 - concentration of reaction products; k_1, k_2, k_3 – stage speed constants [7].

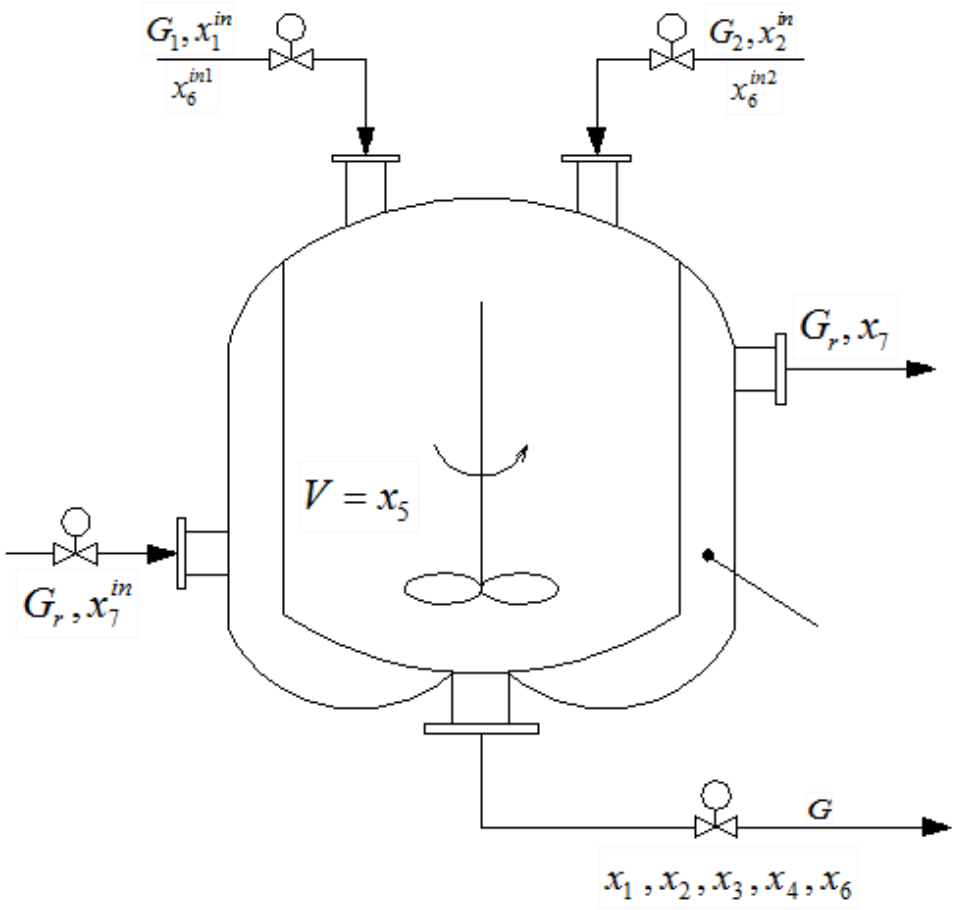

Fig. 1. ***Flow scheme of chemical reactor.***

The apparatus implements a three-stage series-parallel exothermic reaction:

$$A + B \xrightarrow{k_1} C_1,\ A + C_1 \xrightarrow{k_2} C_2,\ A + C_2 \xrightarrow{k_3} C_3 \qquad (7)$$

where *A* and *B* starting reagents; C_1, C_2, C_3 – reaction products; k_1, k_2, k_3 - stage speed constants. The target component is the substance C_2. Starting reagents *A* and *B* with concentrations x_1^{ex}, x_2^{ex} – served in the device in separate streams with costs G_1, G_2 –and temperatures x_6^{ex1}, x_6^{ex2} – respectively. G_{sv} – refrigerant consumption at the inlet and outlet of the apparatus; x_7^{ex}, x_7 – refrigerant temperature at the inlet and outlet of the apparatus; G – mixture consumption at the outlet of the apparatus; x_1, x_2, x_3, x_4 – component concentrations *A*, *B*, C_1, C_2 in the reactor; x_6 – the temperature of the reaction mixture in the apparatus; $V = x_5$ – apparatus volume; G_{sv} – shirt refrigerant volume [8].

The mixture from the reactor is taken by the pump. Since an exothermic reaction proceeds in the apparatus, a coolant is fed into the reactor jacket to cool the reaction mass [9].

A mathematical model of the dynamics of a chemical reactor consists of material balance equations for each component in the reactor, heat balance equations of the reaction mixture and the coolant in the shirt:

$$\begin{cases} \frac{dx_1}{dt} = R_1 + \frac{G_1 \cdot x_1^{in}}{V} - \frac{G \cdot x_1}{V}, \\ \frac{dx_2}{dt} = R_2 + \frac{G_2 \cdot x_2^{in}}{V} - \frac{G \cdot x_2}{V}, \\ \frac{dx_3}{dt} = R_3 - \frac{G \cdot x_3}{V}, \\ \frac{dx_4}{dt} = R_4 - \frac{G \cdot x_4}{V}, \\ \frac{dx_6}{dt} = \frac{G_1 \cdot x_6^{in1}}{V} + \frac{G_2 \cdot x_6^{in2}}{V} - \frac{G \cdot x_6}{V} + \frac{\Delta H_1 \cdot k_1 \cdot x_1 \cdot x_2 + \Delta H_2 \cdot k_2 \cdot x_1 \cdot x_3 + \Delta H_3 \cdot k_3 \cdot x_1 \cdot x_4}{\rho \cdot C} - \frac{K_T \cdot F_T \cdot (x_6 - x_7)}{V \cdot \rho \cdot C} \\ \frac{dx_7}{dt} = \frac{G_r \cdot x_7^{in}}{V_r} - \frac{G_{sv} \cdot x_7^{inp}}{V_r} + \frac{K_T \cdot F_T \cdot (x_6 - x_7)}{V_r \cdot \rho_r \cdot C_r} \end{cases} \quad (8)$$

where $R_1 = -k_1 \cdot x_1 \cdot x_2 - k_2 \cdot x_1 \cdot x_3 - k_3 \cdot x_1 \cdot x_4$, $R_2 = -k_2 \cdot x_1 \cdot x_2$, $R_3 = k_1 \cdot x_1 \cdot x_2 - k_2 \cdot x_1 \cdot x_3 \cdot x_4$, $R_4 = k_2 \cdot x_1 \cdot x_3 - k_3 \cdot x_1 \cdot x_4 -$ is the rate of reaction on components. $\Delta H_i, i = 1,...,3 -$ thermal effect of the corresponding reaction stage; $K_T, F_T -$ heat transfer coefficient through the wall and heat transfer surface of the apparatus; $\rho, C -$ density and heat capacity of the reaction mixture; $\rho_r, C_r -$ density and heat capacity of the refrigerant.

Analysis of the ODE system (8), which describes the dynamics, shows that the object is multidimensional, nonlinear, and multiply connected. Suppose that, based on the conditions of physical feasibility, the flow rate of the input stream of reagent B and the flow rate of the refrigerant, i.e. $u_1 = G_2, u_2 = G_r$.

The system of equations of the model will take the form:

$$\begin{cases} \frac{dx_1}{dt} = R_1 + \frac{G_1 \cdot x_1^{in}}{V} - \frac{G \cdot x_1}{V}, \\ \frac{dx_2}{dt} = R_2 - \frac{G \cdot x_2}{V} + \frac{x_2^{in}}{V} \cdot u_1, \\ \frac{dx_3}{dt} = R_3 - \frac{G \cdot x_3}{V}, \\ \frac{dx_4}{dt} = R_4 - \frac{G \cdot x_4}{V}, \\ \frac{dx_6}{dt} = \frac{G_1 \cdot x_6^{in1}}{V} - \frac{G \cdot x_6}{V} + \frac{\Delta H_1 \cdot k_1 \cdot x_1 \cdot x_2 + \Delta H_2 \cdot k_2 \cdot x_1 \cdot x_3 + \Delta H_3 \cdot k_3 \cdot x_1 \cdot x_4}{\rho \cdot C} - \frac{K_T \cdot F_T \cdot (x_6 - x_7)}{V \cdot \rho \cdot C} + \frac{\cdot x_6^{in2}}{V} \cdot u_1, \\ \frac{dx_7}{dt} = \frac{K_T \cdot F_T \cdot (x_6 - x_7)}{V_r \cdot \rho_r \cdot C_r} + \frac{(x_7^{кир} - x_7)}{V_r} \cdot u_2 \end{cases} \quad (9)$$

The flow of the initial reagent $G_1 -$ at the input to the device is suggested as the control effect for the volume regulation. In addition, one should also choose the control for stabilizing the concentration x_4 at the given degree under the action of disturbances. The analysis of the structure of equations of mathematical model of reactor (8) shows that variables x_1 and x_3 may act as the internal controls and the direct external effect can be performed only on x_1 by the change of the consumption of initial reagent G_1 at the input to reactor. Thus, the control channels of the concentration of the target component and volume of the mixture in the device are represented as follows: $u_1 \to x_1 \to x_4, u_2 \to x_5$, where $u_1 = x_1, u_2 = x_2$ [9].

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. Furthermore, the aim of the motion of system is formulated as the desired invariant manifold in phase space of object, which acts as a target attractor. These and other factors determine the creation of an effective control system, taking into account the features of the current state of the technological process [10].

In general, the problem of synergetic synthesis of the control system is formulated as follows: the control principle, $u=(u_1,..u_m)^T$, should be determined as the function of state variables of object $u_1=(u_1,..u_n),\ ...,u_m=(u_1,..u_n),$ which transforms the representative point of system in phase space from the random initial state to the environment of the given invariant manifolds $\psi_s(x_1...,x_n)=0,\quad s = 1,..., m$ and subsequent motion along the intersection of manifolds to somewhat stationary point or to somewhat dynamic mode [11].

Macro variables $\psi_s(x_1...,x_n)$ must satisfy the functional equation $T_1\dot{\psi}_1(t)+\psi_1(t)=0$, (10) which at $\varphi(\psi)\psi>0$ and $T>0$. Because the mathematical model of object (8) contains two external controlling effects $u_1=G_2$ and $u_2=G_r$, we use the ADAR method on the basis of parallel-series combination of invariant manifolds [13].

Let us introduce aggregate macrovariables to consideration, the first of which determines the relationship of x with controlled variable x and the second reflects the technological requirement to the volume of reaction system as follows

$$\psi_1=x_4-\overline{x_4},\quad \psi_2=x_7+\nu\cdot(x_6) \tag{11}$$

where $\nu(x_6)$ is somewhat function, which should be determined at subsequent procedure of synthesis. Macrovariables (11) should follow the solution of principal functional equation of ADAR method (10).

Let us introduce the macrovariables and of equation (11) to functional equation (10) for the synthesis of control principle, $u=(u_1,..u_m)^T$. As result, we obtain the following equations [14]:

$$T_1\frac{dx_4}{d\tau}+x_4-\overline{x_4}=0,\ \text{and}\ T_2\left[\frac{dx_7}{d\tau}+\frac{\partial\nu_1}{\partial x_6}.\frac{dv_1}{d\tau}\right]+x_7+\nu_7=0. \tag{12}$$

We obtain the following relationships for the control principle from equations (12):

$$u_1=\frac{(x_4-\overline{x_4})}{T_1}+\overline{G}-u_1, \tag{13}$$

$$u_2=\frac{(x_7+\nu_1)x_4}{T_2\cdot x_7^{in}}-\frac{R_1\cdot x_4}{x_7^{in}}-\frac{\overline{G}\cdot x_1}{x_7^{in}}\cdot\frac{\partial\nu_1}{\partial x_6}\cdot\frac{(R_5\cdot x_4-x_5\cdot\overline{G})}{x_1^{in}}$$

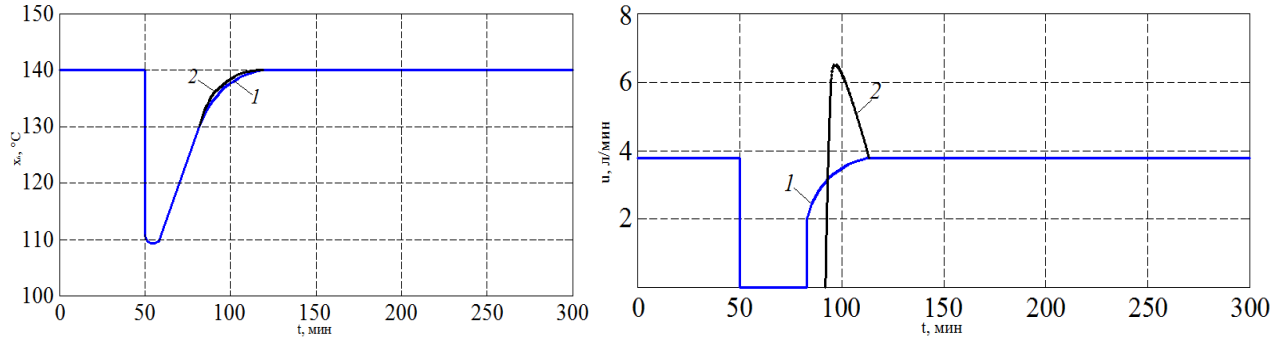

Fig. 2. ***Transients of the output variable and control at the initial deviation of state variables from statics:*** *1 - the first embodiment of the control algorithm, 2 - the second option.*

As a result of simulation it was found that the closed-loop control system does not have a static control error when uncontrolled parametric and signal disturbances act on the object, changes in the set actions and the initial conditions deviate from static values when implementing the version of the control law that provides only for partial measurement of the object state variables. Fault detection schemes which are based on residualgeneration between the measured and some estimated process states require the investigation of mathematical models of the process [15]. Figure 1 shows examples

of transients in a closed system “chemical reactor - non-linear robust controller” with an initial deviation of the state variables of the object, which corresponds to a disturbance in the region of large deviations from the equilibrium state. The deviation of the state variables of the object from the values in statics can be caused by any parametric or signal disturbance, which leads to the exit of the object from the desired equilibrium state [16]. In this case, the control system must ensure the transfer of the object to a given final state, determined by the required temperature.

Conclusion

The problem of analytical synthesis of nonlinear control laws, which stabilizes the temperature and concentration of the process in the chemical reactor by means of synergistic control methods, is solved. Computer simulation of the object-regulator isolated system confirmed these properties of synthesized control system as the ability to switch chemical reactor from one mode of work to another, disturbance invariance, covariance to the given actions, and asymptotic stability. These facts make synergetic control theory very promising applied to such complex, manifold, and nonlinear objects of chemical engineering as chemical reactors. The results of studying the generalized system properties of the object allow solving the synthesis of the control system in various fields. In other words, they allow the formation of different types of topological structure of future management systems.

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