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Analytical Synthesis of Non-Linear Control Algorithms of a Chemical Reactor Thermal Mode

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Abstract: The paper deals with two approaches to the synthesis of a non-linear control system of the thermal regime of a liquid-phase chemical reactor at the realization of a bimolecular exothermic reaction. Synthesis of control algorithms is carried out by the method of analytical design of aggregated regulators (ADAR). The first variant assumes synthesis of temperature controller by classic ADAR method on the basis of a sequential set of invariant manifolds. The second one is based on the cascade control system structure. Computer simulation is used to study and compare the synthesized control systems.

Keywords: chemical reactor; thermal condition; cascade control system; analytical design of aggregated regulators; synergetic control theory; computer simulation

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1. Introduction

The reactor subsystem is a central part of the overall scheme for the transformation of initial reagents into target products and largely determines resource and energy saving, the economic efficiency of the production process as a whole, and the consumer demand for certain products [1].

The purpose of the chemical reactor operation is to provide, by standards, a value of the concentration of the target product at the outlet that determines the quality of the product. In the case of a constant amount of starting reagents, the product concentration value is determined by the process temperature, since it determines the rate at which the starting materials are transformed into reaction products. For this reason, and due to the complexity of real-time concentrations measurement, the process is often performed at temperature and the role of the automatic control system of the object is to stabilize the thermal regime of the process under fault conditions, as well as when transferring an object from one regime to another [2,3].

The main feature of chemical reactors as control objects is their nonlinearity and multi-connectivity, as well as the parametric uncertainty of the reactor mathematical model in the design stage. Until now, the reactor's thermal regime has been controlled in most cases using single-circuit or cascade automatic control systems based on linear Proportional Integral Derivative (PID) algorithms [4,5]. The main drawback of such systems is the problem of maintaining the robustness properties, i.e., maintaining the stability and control quality under the action of parametric disturbances and the transition of the object from one mode to another [6,7], as the synthesis of these systems does not take into account the nonlinearity of the object mathematical model.

In our opinion, the Analytical Design of Aggregated Regulators (ADAR) method, developed as part of synergetic control theory [8–18], which provides asymptotic stability of the automatic control system as a whole in a wide range of changes in state variables and the input variables appear promising in this regard.

Earlier in [17,18], the task of synthesizing a nonlinear algorithm for temperature stabilization using the ADAR method was solved. This paper considers and analyses two alternatives for the synthesis of a nonlinear reactor thermal control system using the ADAR method. The first variant assumes synthesis of the temperature regulator by the classic ADAR method based on a successive set of invariant manifolds. The second one is based on the cascade control system structure.

2. Control Object Description and Control Problem Statement

A liquid-phase chemical reactor is a continuous capacitive device operating in polytropical mode (Figure 1). The apparatus has a bimolecular exothermic reaction $A + B \xrightarrow{k_1} P$,where A and B are the initial substances; P is the reaction product; k_1 is the speed constant. Source reagents A and B are fed into the device in separate streams. The mixture is taken from the reactor by a pump. To remove heat and stabilize the temperature in the reactor, the apparatus is equipped with a jacket, into which the coolant enters.

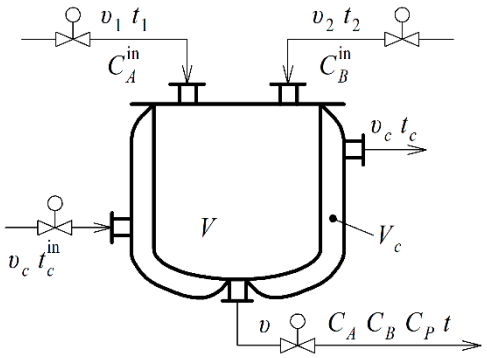


Figure 1. Scheme of the chemical reactor.

In Figure 1, the following nomenclature is used: ${C_A}^{\text{in}}$, ${C_B}^{\text{in}}$ are the concentrations of initial reagents; v_1, v_2 are the flow of initial reagents; t_1, t_2 are the temperatures of initial reagent flows; ${t_c}^{\text{in}}$, t_c are the temperatures of the coolant at the inlet and outlet of the unit, respectively; v_c is the coolant flow at the inlet and outlet of the unit; t is the temperature of the reaction mixture in the apparatus; v is the flow of reaction mixture at the outlet of the apparatus; C_A, C_B, and C_P are the concentrations of components A, B and, P in the reactor, respectively; V is the volume of the reaction mixture in the apparatus; V_c is the volume of the coolant in the jacket.

The mathematical model of the object's dynamics under the assumption of level constancy has the form:

$$\begin{aligned} \frac{dC_A}{d\tau} &= f_1, \\ \frac{dC_B}{d\tau} &= f_2, \\ \frac{dC_P}{d\tau} &= f_3, \\ \frac{dt}{d\tau} &= f_4 + \frac{\beta_1}{V} t_c, \\ \frac{dt_c}{d\tau} &= f_5 + \frac{t_c^{in} - t_c}{V_c} \Delta v_c, \end{aligned} \tag{1}$$

where

$$f_1 = \frac{v_1 \cdot C_A^{in} - (v_1+v_2) \cdot C_A - V \cdot k_1 \cdot C_A \cdot C_B}{V},$$
$$f_2 = \frac{v_2 \cdot C_B^{in} - (v_1+v_2) \cdot C_B - V \cdot k_1 \cdot C_A \cdot C_B}{V},$$
$$f_3 = \frac{V \cdot k_1 \cdot C_A \cdot C_B - (v_1+v_2) \cdot C_p}{V},$$
$$f_4 = \frac{v_1 \cdot t_1 + v_2 \cdot t_2 + \alpha \cdot k_1 \cdot C_A \cdot C_B - (v_1+v_2) \cdot t - \beta_1 \cdot t}{V},$$
$$f_5 = \frac{v_c \cdot (t_c^{in} - t_c) + \beta_2 \cdot (t - t_c)}{V_c},$$
$$\alpha = \frac{V \cdot \Delta H}{\rho \cdot C},$$
$$\beta_1 = \frac{K \cdot F}{\rho \cdot C},$$
$$\beta_2 = \frac{K \cdot F}{\rho_c \cdot C_c},$$
$$k_1 = k_1^0 \cdot \exp\left[\frac{-E_1}{R(t+273)}\right],$$

and where k_1 is the speed constant; k_1^0 is the pre-exponential multiplier of the rate constant; E_1 is the activation energy; R is the universal gas constant; ΔH is the heat effect of the reaction; ρ and C are the density and heat capacity of the reaction mixture, respectively; ρ_c and C_c are the coolant density and heat capacity, respectively; K is the heat transfer coefficient; F is the heat exchange surface; Δv_c is the deviation of the coolant flow from the nominal value.

The general task of the chemical reactor control is to stabilize the mixture temperature in the apparatus at a given level, $\bar{t}$, under conditions of disturbances. The control activity is the coolant flow rate fed into the jacket.

2.1. Control Algorithm Synthesis by the ADAR Method Based on a Sequential Set of Invariant Manifolds

Since the mathematical model of the object, Equation (1), contains one external control action $u = \Delta v_c$, it is necessary to use the ADAR method based on a sequential set of invariant manifolds [8]. The analysis of Equation (1) shows that the control action $u = \Delta v_c$ affects the variable t through the variable t_c. Thus, the control channel for the temperature of the mixture in the apparatus will be written in full form $u \to t_c \to t$. According to the ADAR method [8,19], it is possible to create a number of manifolds in the phase space of dynamic systems, to which phase trajectories are attracted.

Hence, it is possible to construct such a set of attracting invariant manifolds $\psi_1(\overline{x}) = 0$, where s is from 1 to m, where the depicting point of the system, having started moving from an arbitrary initial position in the phase space, moves sequentially from one manifold to another until it reaches the last one $\psi_m(\overline{x}) = 0$, resulting in a given final state. In this way, the depicting point first approaches the manifold $\psi_1(\overline{x}) = 0$, then the manifold $\psi_2(\overline{x}) = 0$, etc. When using m attracting manifolds, the dimension of each i^{th} manifold will be one unit smaller than the previous one, which results in phase volume compression and dynamic decomposition of the task.

A qualitative analysis of the structure of the right parts of the system Equation (1) shows that the state variables are interconnected (e.g., there are other phase coordinates in the right part of the equation for t).

Based on this fact, and the principle of control equivalence, we will introduce the invariant manifold:

$$\psi_1 = t_c + v(t) = 0, \quad (2)$$

where $v(t)$ is the unknown function of t. The control law is synthesized in such a way that the system's depicted point in the phase space is transferred from an arbitrary start position

to the neighborhood of manifold $\psi_1 = 0$. A change in the aggregated macro variable that plays the role of an order parameter shall be subject to the functional equation:

$$T_1 \cdot \psi_1 + \psi_1 = 0, \tag{3}$$

where value T_1 (and T_2 in other equations) are algorithm tuning parameters. Equation (3), taking into account Equation (2), takes the following form:

$$T_1 \left[\frac{dt_c}{d\tau} + \frac{\partial v}{\partial t} \cdot \frac{dt}{d\tau} \right] = -\psi_1.$$

Due to equations of the object, Equation (1), this expression will be written down:

$$T_1 \left[f_5 + \frac{\left(t_c^{in} - t_c\right)}{V_c} u + \frac{\partial v}{\partial t} \left[f_4 + \frac{\beta_1}{V} \cdot t_c \right] \right] + t_c + v = 0, \tag{4}$$

where $u = \Delta v_c$. From Equation (4) we obtain an expression for the control algorithm:

$$u = -\frac{V_c(t_c + v)}{T_1\left(t_c^{in} - t_c\right)} - \frac{\partial v}{\partial t} \cdot \frac{\left(f_4 + \frac{\beta_1}{V} t_c\right) \cdot V_c}{t_c^{in} - t_c} - \frac{f_5 \cdot V_c}{t_c^{in} - t_c}. \tag{5}$$

The control action u transfers the depicting point of the system to the neighborhood of manifold $\psi_1 = 0$, where the link $t_c = -v$ is implemented and the effect of 'phase space compression' is realized, i.e., there is a decrease in the dimension of the system of Equation (1). The equations of the decomposed system taking into account the relation $t_c = -v$ will take the form:

$$\begin{aligned} \tfrac{dC_A}{d\tau} &= f_1, \\ \tfrac{dC_B}{d\tau} &= f_2, \\ \tfrac{dC_p}{d\tau} &= f_3, \\ \tfrac{dt}{d\tau} &= f_4 - \tfrac{\beta_1}{V} \cdot v. \end{aligned} \tag{6}$$

The function $v(t)$ in the decomposed system, Equation (6), can be regarded as an 'internal' control that moves the object, Equation (6), along manifold $\psi_1 = 0$. In the second step of the control law synthesizing procedure, the expression for $v(t)$ is searched. The purpose of the system movement, Equation (6), is introduced in the form of an invariant manifold which represents a technological requirement of the system:

$$\psi_2 = t - \bar{t} = 0. \tag{7}$$

Macro variable ψ_2 satisfies the solution of the functional equation $T_2 \cdot \psi_2 + \psi_2 = 0$ which, taking into account the expression, Equation (7), due to the decomposed system model, Equation (6), will take the form:

$$T_2 \left(f_4 - \frac{\beta_1}{V} v \right) + t - \bar{t} = 0. \tag{8}$$

'Internal' control action according to Equation (8) will be written down

$$v = \frac{\left(t - \bar{t}\right) \cdot V}{T_2 \cdot \beta_1} + \frac{f_4 \cdot V}{\beta_1}. \tag{9}$$

Control law, Equation (9), ensures that the depicted point is asymptotically close to the second attracting manifold $\psi_2 = t - \bar{t} = 0$. The final expression for the external control law u can be obtained by substituting in Equation (5), the function v and its partial derivative $\partial v / \partial t$.

The control law tuning parameters, which affect the quality of the process dynamics in an isolated object-regulator system, are the time constants T_1, T_2. The asymptotic stability conditions of the system as a whole with respect to the manifolds $\psi_1 = 0$, $\psi_2 = 0$ introduced into the phase space have the form: $T_1 > 0$, $T_2 > 0$ [8].

2.2. Synthesis of a Cascade Thermal Control System

The structural and technological features of the chemical reactor, the specific conditions of the complex technological process implementation, and, accordingly, the structural features of the mathematical model, Equation (1), allow decomposition of the system, Equation (1), into two subsystems. The first subsystem is the material balance equation by component and the thermal balance equation of the reaction mixture. The temperature of the coolant in the jacket is a control action for the temperature of the mixture in the tank. The second subsystem is the reactor jacket, the functioning of which is described by the thermal equilibrium equation, and the state is characterized by the coolant temperature t_c. The control for t_c is the coolant flow rate v_c. The object structural diagram is shown in Figure 2.

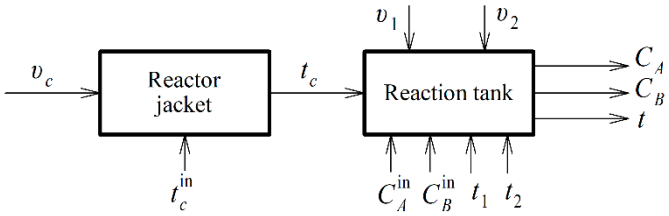


Figure 2. Structural diagram of the control object.

Cascade control systems are widely used in the linear automatic control theory and the automation practice of objects with such structure [20]. We will solve the problem of synthesis of the cascade control system of temperature in the reactor by the methods of synergistic control theory. The mathematical model of the perturbed movement of the first subsystem will take the form:

$$\begin{aligned} \tfrac{dC_A}{d\tau} &= f_1, \\ \tfrac{dC_B}{d\tau} &= f_2, \\ \tfrac{dC_p}{d\tau} &= f_3, \\ \tfrac{dt}{d\tau} &= f_4 + \tfrac{\beta_1}{V} \cdot u_1, \end{aligned} \tag{10}$$

where $u_1 = t_c$.

The task is formulated as follows. It is necessary to synthesize the control law u_1, which transfers an object from an arbitrary starting position to the neighborhood of a given invariant manifold $\psi_1 = 0$ and ensures stable movement along $\psi_1 = 0$ to a final state. This problem is solved in one step, as the control is directly included in the temperature equation for the reaction mixture [8].

Let us introduce the macro variable ψ_1:

$$\psi_1 = t - \bar{t},$$

where $\bar{t}$ is the set temperature point. The control action must be such that the change in the macro variable ψ_1 is subject to the basic functional equation:

$$T_1 \cdot \dot{\psi}_1 + \psi_1 = 0.$$

We will write this equation in full form due to the equations of the model, Equation (10):

$$f_4 + \frac{\beta_1}{V} \cdot u_1 = -\frac{1}{T_1}(t - \bar{t}).$$

From here we obtain:

$$u_1 = -\frac{V}{T_2 \cdot \beta_1}(t - \bar{t}) - \frac{f_4 \cdot V}{\beta_1}. \tag{11}$$

The algorithm tuning parameter is the value T_1. A condition of asymptotic stability of the closed-loop control subsystem of the reaction tank is $T_1 > 0$.

Another step in the synthesis of the temperature control system is the synthesis of the algorithm for controlling the coolant temperature t_c. The task of the subsystem which controls the coolant temperature in the jacket is to define such external control Δv_c, which would provide the coolant temperature value $\bar{t}_{xl} = u_1$ defined at the first stage. The model of the subsystem is as follows:

$$\frac{dt}{d\tau} = f_5 + \frac{(t_c^{in} - t_c)}{V_c} u_2, \tag{12}$$

where $u_2 = \Delta v_c$.

In terms of the ADAR method, the task of synthesizing the coolant temperature control algorithm is formulated as follows. It is necessary to synthesize the control law u_2, which transfers the object from an arbitrary starting position to the neighborhood of the manifold $\psi_2 = 0$ and provides stable movement to a given final state.

The attracting invariant manifold will be written down:

$$\psi_2 = t_c - u_1 = 0.$$

Using the functional equation $T_2 \cdot \dot{\psi}_2 + \psi_2 = 0$ and Equation (12), we will obtain the control law:

$$u_2 = -\frac{V_c}{T_2(t_c^{in} - t_c)}(t_c - u_1) - \frac{f_5 \cdot V_c}{t_c^{in} - t_c}. \tag{13}$$

The algorithm tuning parameter is the T_2. A condition of asymptotic stability of the reactor jacket closed control subsystem is $T_2 > 0$.

Based on the type of Equations (11) and (13), the structure of the cascade control system without parametric perturbations can be presented as follows (Figure 3).

By substituting u_1 from Equations (3)–(5), we obtain a control law for the auxiliary regulator that defines the value of the external control action:

$$u_2 = -\frac{V_c}{T_2(t_c^{in} - t_c)}\left[t_c + \frac{V}{T_2 \cdot \beta_1}(t - \bar{t}) + \frac{f_4 \cdot V}{\beta_1}\right] - \frac{f_5 \cdot V_c}{t_c^{in} - t_c}. \tag{14}$$

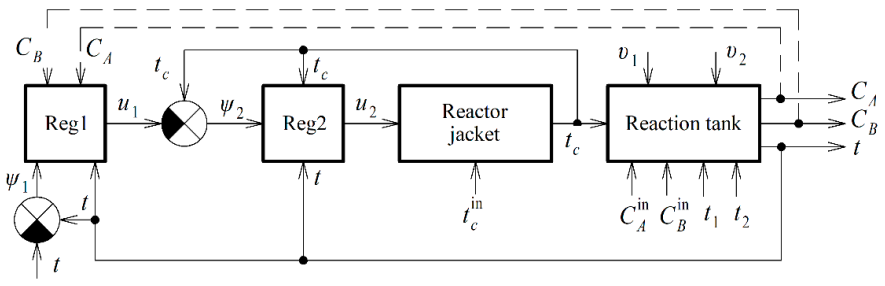


Figure 3. Structure of the cascade reactor thermal control system: Reg1—main controller; Reg2—auxiliary control system.

2.3. Computer Simulation of the Control System

The performance of the thermal control system of the chemical reactor using the synthesized nonlinear laws, Equations (5), (9), and (14) was examined by computer simulation methods. The properties of perturbation invariance, covariance with temperature set points, and asymptotic stability of the closed system were studied.

Simulation was carried out at technological and structural parameters ensuring optimal operation mode of the chemical reactor [21,22]:

- V = 500 L, V_c = 290 L;
- ${C_A}^{\text{in}}$ = 19.74 mol/L, ${C_B}^{\text{in}}$ = 10.93 mol/L;
- v_1 = 1.5 L/min, v_2 = 3.5 L/min, v = 5 L/min, v_c = 3.84 L/min;
- t_1 = 20 °C, t_2 = 30 °C, ${t_c}^{\text{in}}$ = 20 °C;
- K = 12 kJ/(m^2·min·K), F = 2.9 m^2;
- ρ = 0.9 kg/L, ρ_c = 1 kg/L;
- C = 2 kJ/(kg·K), C_c = 4.18 kJ/(kg·K);
- ΔH = 80 kJ/mol, E_1 = 48635 J/mol, ${k_1}^0$ = 109860 l/(mol·min).

The parameters of control laws are as follows: time constants values $T_1 = T_2$ = 20 min (determined from the time requirements of the control process); set point of reactor mixture temperature $\bar{t} = 140$ °C.

Figures 4 and 5 show examples of control transients in a closed system under an initial deviation of all state variables from the statics by −20% ($\Delta C_A = -0.2 \cdot {C_A}^0$, $\Delta C_B = -0.2 \cdot {C_B}^0$, $\Delta C_P = -0.2 \cdot {C_P}^0$, $t = -t^0$, $t_c = -0.2 \cdot {t_c}^0$) and at a step change in the set point value ($\Delta\bar{t} = -10$°C). For clarity, the transients before applying the input action (τ = 50 min) are given in a static mode. In the first variant, the value of the control effect Δv_c is calculated using Equations (5) and (9), and in the second one using Equation (14). The figures show that the quality indicators of the proposed control systems with identical control settings are close.

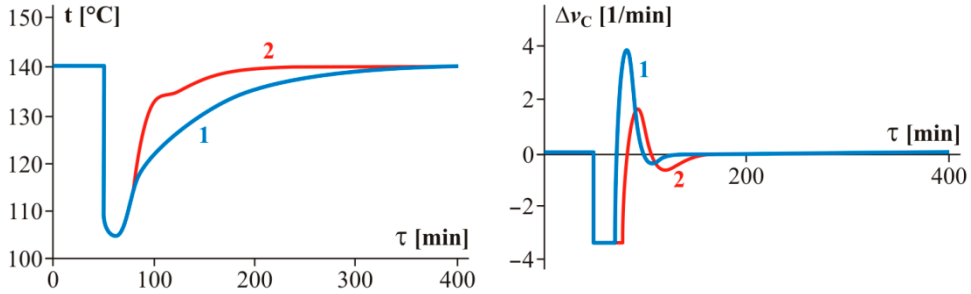


Figure 4. Transients in a closed system with an initial deviation of the state vector from static by −20%: 1—the first variant of the algorithm (classic ADAR method); 2—second variant (cascade control system).

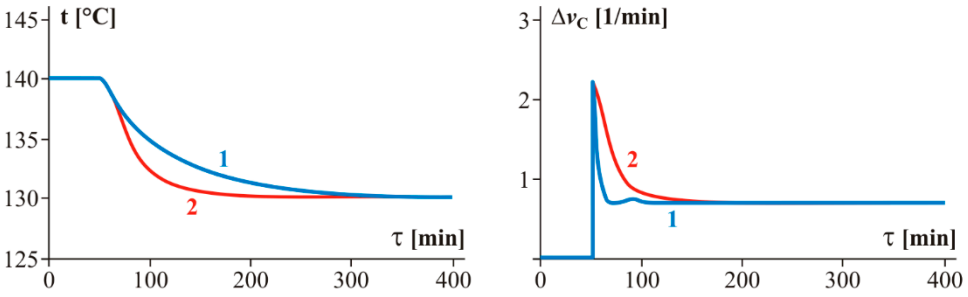


Figure 5. Transients in a closed system with a step change in temperature set point by −10 °C: 1—the first variant of the algorithm (classic ADAR method); 2—second one (cascade control system).

3. Conclusions

The paper considers possible approaches to the synthesis of a nonlinear thermal control system of a liquid-phase chemical reactor using the ADAR method. Temperature control algorithms were obtained using a nonlinear mathematical model of the object without using the linearization procedure. This fact is a significant advantage in the synthesis of an automatic control system in the design stage in the case of a real control object absence.

The principal difference between the approach to the synergistic synthesis of a cascade automatic control system for reactor thermal control and the classical approach (ADAR method based on a sequential set of invariant manifolds) is as follows. The classical ADAR method implements a cascade synthesis of the automatic control system, in which a dynamic decomposition of the model takes place with the decrease in its dimensionality per unit after the first stage of synthesis (defining the external control that transfers the object to the first invariant manifold). In the second stage, the law of internal control change is defined, which ensures that the object moves along the first manifold to the final state. The proposed approach preliminarily decomposes the object and therefore the dynamic model into two related subsystems. In the first stage, the internal control is defined, which transfers the object to the specified final state, and in the second phase, the external control is defined, which provides the evaluated value of the internal control.

In general, both variants of the synthesized automatic thermal control systems are operable and can be recommended for any type of reaction.

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