

Simulation of Catalytic Processes in a Fixed Bed with the Use of Microwave Radiation for Performing an Endothermic Reaction

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Abstract—A quasi-homogeneous model of a catalytic fixed-bed reactor, in which an endothermic chemical reaction occurs with the use of microwave radiation energy, was proposed and numerically analyzed. The versions of the arrangement of a radiation source at the reactor inlet and outlet and also the versions of microwave radiation energy conversion into heat by a catalyst and an initial gaseous reagent were considered. The effects of model parameters on the dynamic behavior of the system were studied, and a qualitative structural difference between the resulting steady-state conditions was demonstrated. The phenomenon of endothermic chemical reaction autowave propagation was discovered, and the regularities of this propagation were studied.

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INTRODUCTION

The great capabilities of microwave radiation in chemistry have generated great interest in the study and application of the resulting effects on a global scale. Interest in new nontraditional technologies based on catalytic processes with the use of microwave radiation, in particular, endothermic heterophase catalytic reactions, has quickened [1–5]. On the traditional heating of a sample, heat transfer is due to thermal conductivity, convection, and thermal radiation, and it is always associated with a temperature gradient. The heating of a sample by microwave radiation is caused by the interaction of this radiation with molecules (ions) within the entire volume of the irradiated material. The depth of microwave radiation penetration in the bulk of the sample is different for different materials. The currently available theory does not make it possible to calculate the portion of the initial microwave radiation energy absorbed by the sample and consumed for its heating (this value is usually referred to as losses). Therefore, the value of losses for a particular substance is determined experimentally. Note that this value changes by a factor of thousands for different substances. The maximally complete absorption of microwave radiation energy in technological processes is a necessary condition for effective energy consumption. For efficiently performing endothermic heterophase catalytic reactions, the diameter and height of a catalyst bed, the feed space velocity, and the power of a microwave generator should be chosen so that the total microwave energy would be converted into thermal energy. The conditions of industrial chemical-engineering processes mainly depend on a tendency to reach a maximum

output of an aggregate at minimum material expenditures. Traditionally, these conditions were restricted by a requirement that all of the process parameters should be constant in time. It is obvious that the design characteristics of a reactor, its productivity, and the activity and grain diameter of a catalyst are determined by the economic efficiency of the process as a whole. It is well known that the mathematical simulation of chemical reactors is used for solving these problems [6, 7].

The aim of this work was to mathematically simulate a catalytic process in a fixed bed with an endothermic chemical reaction, which occurs due to microwave energy absorption, and to study the effect of model parameters on changes in the main performance characteristics of the process.

MATHEMATICAL MODEL

A fixed bed of a catalyst is a complex system with an inevitable statistical distribution of properties in individual structural elements. The irregularity of dispersity in a heterogeneous medium, the turbulization of flows, and other factors makes the system more complicated. The equations of mathematical physics serve as a theoretical support and prototype for the development and optimization of catalytic processes, but the macroscopic parameters of these equations play the role of effective values unlike the classical equations of mathematical physics for continuous media. The construction, selection, and simplification of models depend on a number of requirements imposed on these models [6, 7].

A mathematical model of unsteady-state processes in the fixed bed of a catalyst in the simplest formulation (in the approximation of a porous medium as two

interpenetrating continua) describes autowave processes in heterogeneous media [8]. This quasi-homogeneous model considers the convective stream of a reaction gas mixture through the catalyst bed, the effective thermal conductivity of a blown granular layer, the chemical conversion of substances, and the generation of heat. The heat- and mass-transfer processes in a catalyst grain are assumed intense so that the concentration and temperature differences between the gas and the catalyst (both on the surface and inside) can be ignored. The gas flow with a negligibly small pressure gradient is considered, and it is believed that the reaction mixture obeys the ideal gas law. On the action of microwave radiation on the system, the quasi-homogeneous model must be supplemented with the fourth subsystem, which takes into account the local heating of the medium. Then, if a reversible chemical reaction like $A \rightleftharpoons B + q$ occurs in the catalyst bed, the mathematical description takes the form

$$(\varepsilon_g \rho_g c_g + \varepsilon_c \rho_c c_c) \frac{\partial T}{\partial t} = \lambda_{\text{eff}} \frac{\partial^2 T}{\partial l^2} - \rho_g u c_g \frac{\partial T}{\partial l} + q C_0 w(T, x) + Q_{\text{microwave}}(l), \quad (1)$$

$$\varepsilon_g \frac{\partial x}{\partial t} = -u \frac{\partial x}{\partial l} + w(T, x), \quad (2)$$

with the boundary conditions

$$l = 0: \lambda_{\text{eff}} \frac{\partial T}{\partial l} = 0, \quad x = x_0, \quad (3)$$

$$l = L: \lambda_{\text{eff}} \frac{\partial T}{\partial l} = 0, \quad (4)$$

and the initial conditions

$$T = 0: T(0, l) = T_i, \quad x(0, l) = x_i. \quad (5)$$

Here, $C_0 = C_{A,0} + C_{B,0}$; $C_{A,0}$ and $C_{B,0}$ are the concentration of reagents A and B at the point of entry into the catalyst bed, respectively; C_B and $x = C_B/C_0$ are the dimensional concentration and the weight (molar) fraction of the product (at $x_0 = (C_{B,0}/C_0) \rightarrow 0$, it is equal to the conversion of reagent A), respectively; c_g and c_c are the heat capacities of the gas and the catalyst, respectively; T_0 , T , and T_i are the inlet, current, and initial temperatures, respectively; t is time; u is the reagent flow rate through the entire cross section of the catalyst bed; l and L are the longitudinal coordinate and the catalyst bed length, respectively; q is the heat effect of the reaction; $Q_{\text{microwave}}(l)$ is the microwave energy converted into the thermal energy of the system; ε and ε_p are the porosities of the catalyst bed and grain, respectively; $\varepsilon_g = \varepsilon + (1 - \varepsilon)\varepsilon_c$, and $\varepsilon_c = 1 - \varepsilon_g$ are the volume fractions of the gas and solid phases,

respectively; λ_{eff} is the effective coefficient of the longitudinal thermal conductivity of the catalyst bed; and ρ_g and ρ_c are the densities of the gas and the catalyst, respectively.

The rate of the reversible first-order chemical reaction $A \rightleftharpoons B$ is described by the expression [9]

$$w(T, x) = \bar{w} - \tilde{w} = \bar{w} \left(1 - \frac{\tilde{w}}{\bar{w}} \right) = k_0 \exp \left(-\frac{E}{RT} \right) (1 - x) \times \left[1 - \frac{x}{(1 - x) K_p(T)} \right], \quad (6)$$

where $K_p(T) = \exp \left(-\frac{\Delta G_T^0}{RT} \right) = \exp \left(-\frac{\Delta H_T^0}{RT} + \frac{\Delta S_T^0}{R} \right) = k \exp \left(\frac{q}{RT} \right)$ is the equilibrium constant of the reaction; E is the activation energy; k_0 and k are the preexponential factors of the rate constant and the equilibrium constant, respectively; ΔG_T^0 , ΔH_T^0 , and ΔS_T^0 are the Gibbs energy, enthalpy, and entropy of the reaction at a standard pressure, respectively; and R is the gas constant.

It is well known that the attenuation of electromagnetic radiation upon its propagation in an absorbing medium is described by the Bouguer–Lambert–Beer law $I(S) = I_0 \exp(-k_\lambda S)$, where I_0 is the entering beam intensity; l_s and S are the longitudinal coordinate and the thickness of the substance layer through which radiation is passed; $k_\lambda = \chi_\lambda C_i$ is the absorption coefficient; χ_λ is a coefficient independent of C_i , which characterizes the interaction of the molecule of the absorbing material with radiation with the wavelength λ ; and C_i is the concentration of the absorbing material. Then,

$$Q_{\text{microwave}}(l) = \frac{dI}{dl} = -k_\lambda(l_s) I_0 \exp \left(-\int_0^S k_\lambda(l_s) dl_s \right) \frac{dl_s}{dl} = -\chi_\lambda C_i(l_s) I_0 \exp \left(-\chi_\lambda \int_0^S C_i(l_s) dl_s \right) \frac{dl_s}{dl}. \quad (7)$$

The energy of microwave radiation can be absorbed by both the catalyst and gaseous substances, for example, water molecules. Most frequently, the catalyst concentration in the reactor is constant; then, the absorption coefficient is constant: $k_\lambda = \text{const}$. At the same time, note that the catalyst concentration in the reactor (the porosity of the catalyst bed and grain) can change over a wide range because it depends on the technological process; therefore, the absorption coefficient can vary. If the gaseous substance that absorbs microwave radiation is a reactant, its concentration changes in the course of reaction, and the absorption coefficient is a variable quantity in this case.

Problem (1)–(5) with consideration for (6) and (7) takes the form

$$(\varepsilon_g \rho_g c_g + \varepsilon_c \rho_c c_c) \frac{\partial T}{\partial t} = \lambda_{\text{eff}} \frac{\partial^2 T}{\partial l^2} - \rho_g u c_g \frac{\partial T}{\partial l} + q C_0 k_0 \exp\left(-\frac{E}{RT}\right) (1-x) \left[1 - \frac{x}{(1-x) K_p(T)}\right] \quad (8)$$

$$- \chi_\lambda C_0 (1-x) I_0 \exp\left(-\chi_\lambda C_0 \int_0^s (1-x) dl_s\right) \frac{\partial l_s}{\partial l},$$

$$\varepsilon_g \frac{\partial x}{\partial t} = -u \frac{\partial x}{\partial l} + k_0 \exp\left(-\frac{E}{RT}\right) (1-x) \times \left[1 - \frac{x}{(1-x) K_p(T)}\right], \quad (9)$$

with the boundary conditions

$$l = 0: \lambda_{\text{eff}} \frac{\partial T}{\partial l} = 0, \quad x = x_0, \quad (10)$$

$$l = L: \lambda_{\text{eff}} \frac{\partial T}{\partial l} = 0 \quad (11)$$

and the initial conditions

$$T = 0: T(0, l) = T_i, \quad x(0, l) = x_i. \quad (12)$$

The radiation source can be placed both at the inlet ($l_s = l$) and at the outlet of the catalyst bed ($l_s = L - l$).

RESULTS AND DISCUSSION

Problem (8)–(12) was solved numerically; differential Eqs. (8) and (9) were approximated by difference equations; the obtained system of linear algebraic equations was solved by the sweep method. The calculations were performed at the following characteristic parameter values: $c_g = 300 \text{ cal kg}^{-1} \text{ K}^{-1}$; $c_c = 249 \text{ cal kg}^{-1} \text{ K}^{-1}$; $E = 35 \text{ kcal mol}^{-1} \text{ K}^{-1}$; $q = -15 \text{ kcal/mol}$; $\lambda_{\text{eff}} = 0.2 \text{ cal m}^{-1} \text{ s}^{-1} \text{ K}^{-1}$; $C_0 = 46.43 \text{ mol/m}^3$; $T_0 = 373 \text{ K}$; $k = 1.743 \times 10^6$; $k_0 = 1.178 \times 10^9 \text{ s}^{-1}$; $p = 1 \text{ atm}$; $\rho_g = 1.3 \text{ kg/m}^3$; $u = 1 \text{ m/s}$; $\rho_c = 2700 \text{ kg/m}^3$; $\varepsilon = 0.42$; and $\varepsilon_p = 0.3$. It is well known that the penetration depth of microwave radiation in the catalyst bed can be as large as tens of centimeters [2]. Based on these data, the value of k_λ was estimated. Because the length of the catalyst bed is greater than the penetration depth of microwave radiation, the heating of the catalyst along the bed (microwave energy conversion into thermal energy) is nonuniform; therefore, it depends on the site of the supply of microwave energy. We consider below two versions of radiation energy supply when the radiating antenna, which is responsible for the uniformity of energy distribution over the cross section of the catalyst bed, is located at the inlet or outlet of the catalyst bed.

Let us consider the case when microwave energy is converted into thermal energy only by the catalyst material; that is, $k_\lambda = \text{const}$ and the radiation source is located at the outlet of the catalyst bed ($l_s = L - l$). Figure 1 shows the dynamics of temperature changes

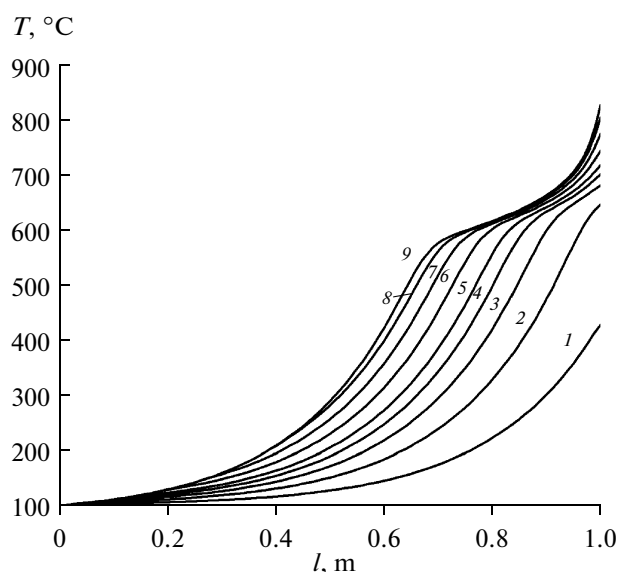


Fig. 1. Dynamics of temperature changes in the catalyst bed at the absorption coefficient $k_\lambda = 5$ and the radiation intensity $I_0 = 970 \text{ kcal m}^{-2} \text{ s}^{-1}$ at different points in time t , s: (1) 20, (2) 40, (3) 60, (4) 80, (5) 100, (6) 140, (7) 200, (8) 300, and (9) 500. The radiating antenna is arranged at the catalyst bed outlet.

along the catalyst bed at the absorption coefficient $k_\lambda = 5$ and the radiation intensity of the microwave generator $I_0 = 970 \text{ kcal m}^{-2} \text{ s}^{-1}$. This radiation intensity leads to the integral heat release in the catalyst bed that compensates the heating of the reaction mixture to a high temperature and energy consumption for the complete occurrence of an endothermic chemical reaction. As can be seen in Fig. 1, the reactor was heated nonuniformly and most intensely near the radiating antenna. At a temperature of about 600°C or higher, the occurrence of the endothermic reaction becomes noticeable, and the temperature profile becomes more gently sloping in a region forward the gas flow. As the reaction is complete, the temperature at the outlet of the catalyst bed intensely increases once again. Approximately 600 s after the onset of the operation of the microwave generator, steady-state conditions are established in the reactor with the outlet temperature of 828.4°C and the conversion $x = 0.9761$. Figure 2 shows the steady-state temperature profiles and the degrees of reactant conversion for three different values of the absorption coefficient $k_\lambda = 3, 5$, and 10 at the radiation intensity $I_0 = 10^6 \text{ cal m}^{-2} \text{ s}^{-1}$. As can be seen in Fig. 2, the smaller the absorption coefficient, the more gently sloping the temperature profile; the maximum temperature decreases (the temperature at the outlet of the catalyst bed) to the values of $T_{\text{out}} = 797.5, 872.9$, and 897.7°C , respectively. In this case, the following degrees of conversion at the outlet of the catalyst bed were obtained: $x_{\text{out}} = 0.9746, 0.9925$, and 0.9872 . The greatest conversion was observed at $k_\lambda = 5$. This extremal function was due to

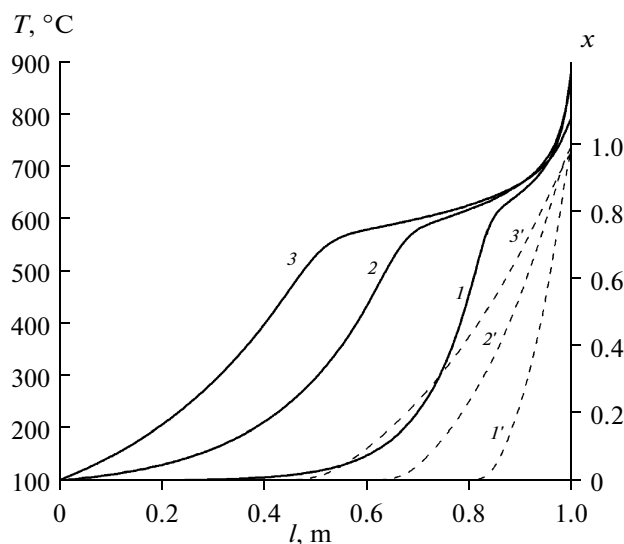


Fig. 2. Steady-state temperature profiles (solid lines) and reactant conversions (dashed lines) at the radiation intensity $I_0 = 10^6 \text{ cal m}^{-2} \text{ s}^{-1}$ for the following three absorption coefficients k_λ : (1, 1') 10, (2, 2') 5, and (3, 3') 3. The radiating antenna is arranged at the catalyst bed outlet.

the fact that the temperature, the equilibrium conversion, and the rate of reaction increase with increasing k_λ ; at the same time, the contact time decreases at high temperatures.

Next, let us consider the case when the radiating antenna is located at the inlet of the catalyst bed ($l_s = l$). Figure 3 shows the dynamics of the temperature change and the conversion along the catalyst bed at $k_\lambda = 5$ and the radiation intensity $I_0 = 10^6 \text{ cal m}^{-2} \text{ s}^{-1}$. Figure 4 shows the distribution functions of the rate of endothermic chemical reaction and heat release along the catalyst bed. On the arrangement of the radiating antenna at the inlet of the catalyst bed, a steeper temperature gradient was observed and the catalyst bed was heated over a much larger region than in the preceding case. Therefore, at the same values of the absorption coefficient $k_\lambda = 3, 5$, and 10 at the outlet of the catalyst bed, the degrees of conversion were higher ($x_{\text{out}} = 0.9986, 0.9995$, and 0.9995) and the temperatures were lower ($T_{\text{out}} = 743.7, 844.6$, and 842.7°C) than in the above case. An increase in the radiation intensity to $I_0 = 1.03 \times 10^6 \text{ cal m}^{-2} \text{ s}^{-1}$ at $k_\lambda = 5$ led to an increase in the conversion $x_{\text{out}} = 0.9997$ and the temperature $T_{\text{out}} = 920.1^\circ\text{C}$. A decrease in the radiation intensity to $I_0 = 970 \text{ kcal m}^{-2} \text{ s}^{-1}$ at $k_\lambda = 5$ led to a decrease in the conversion $x_{\text{out}} = 0.9992$ and the temperature $T_{\text{out}} = 769.3^\circ\text{C}$ at the catalyst bed outlet. Thus, a change in the location of the radiating antenna from the outlet to the inlet of the catalyst bed led to qualitative changes in dynamic and steady-state conditions.

Let us consider the case when the catalyst does not interact with microwave radiation and the main

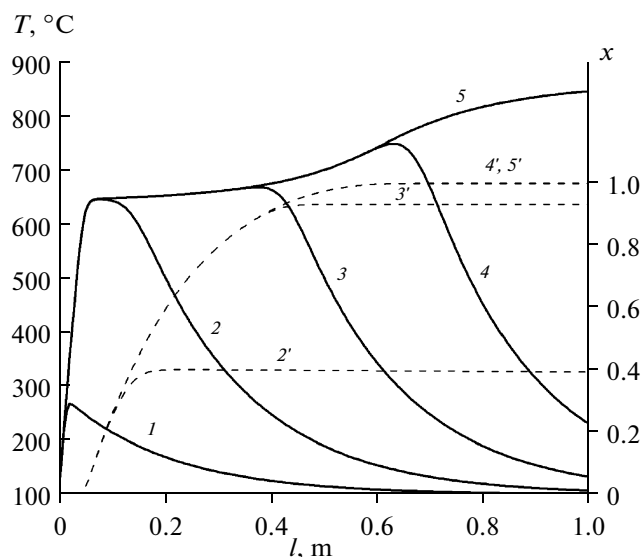


Fig. 3. Dynamics of (solid lines) temperature and (dashed lines) conversion changes in the catalyst bed at $k_\lambda = 5$ and the radiation intensity $I_0 = 10^6 \text{ cal m}^{-2} \text{ s}^{-1}$ at different points in time t , s: (1) 10, (2) 50, (3) 150, (4) 300, and (5) 1000. The radiating antenna is arranged at the catalyst bed inlet.

amount of radiant energy is converted into thermal energy by a reactant, for example, by water molecules, whose concentration decreases in the course of the reaction. This will lead to a decrease in the absorption coefficient k_λ of the medium in the course of the reaction. As in the above case, we consider two versions of energy supply when the radiating antenna, which is responsible for the uniform energy distribution over the catalyst bed cross section, is arranged at the inlet or outlet of the catalyst bed.

Figure 5 shows the dynamics of temperature changes along the catalyst bed at $\chi_\lambda = 0.323$ and the radiation intensity $I_0 = 10^6 \text{ cal m}^{-2} \text{ s}^{-1}$ in the case when the radiating antenna is located at the outlet of the catalyst bed ($l_s = L - l$). As can be seen in Fig. 5, the wave of endothermic chemical reaction with a steep temperature gradient in the front propagates through the catalyst bed in the opposite direction to the gas flow. The process becomes a steady-state process after the reaction front reaches the left boundary of the catalyst bed because the further propagation of the wave is impossible. In this case, the temperature at the catalyst bed outlet is $T_{\text{out}} = 740.1^\circ\text{C}$ and the conversion is $x_{\text{out}} = 0.9990$. A decrease in the radiation intensity to $I_0 = 970 \text{ kcal m}^{-2} \text{ s}^{-1}$ led to a small decrease in the temperature and the conversion at the catalyst bed outlet: $T_{\text{out}} = 736.0^\circ\text{C}$ and $x_{\text{out}} = 0.9990$. An increase in the catalyst bed length does not lead to a change in the qualitative behavior of the system. As the rate of gas filtration increases to $u = 1.2 \text{ m/s}$, the effective thermal conductivity of the catalyst bed cannot ensure the propagation of a reaction front in the opposite direction to the gas flow, and the catalyst bed is cooled by

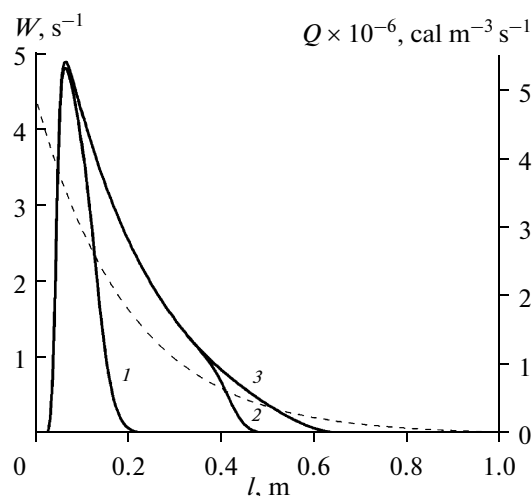


Fig. 4. Distribution functions of (solid lines) the rate of endothermic chemical reaction and (dashed lines) heat release along the catalyst bed at $\chi_\lambda = 5$ and the radiation intensity $I_0 = 10^6 \text{ cal m}^{-2} \text{ s}^{-1}$ at different points in time t , s: (1) 50, (2) 150, and (3) 300 (correspond to curves 2–4 in Fig. 3, respectively). The radiating antenna is arranged at the catalyst bed inlet.

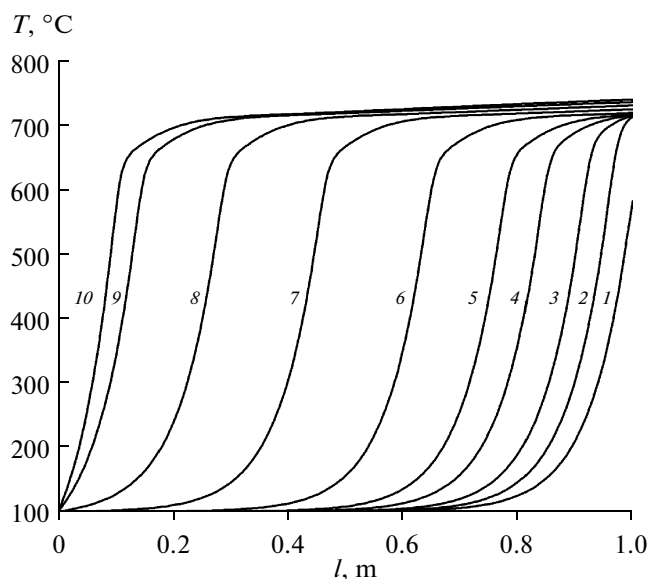


Fig. 5. Dynamics of temperature changes in the catalyst bed at $\chi_\lambda = 0.323$, the radiation intensity $I_0 = 10^6 \text{ cal m}^{-2} \text{ s}^{-1}$, and $u = 1 \text{ m/s}$ at different points in time t , s: (1) 10, (2) 20, (3) 40, (4) 100, (5) 200, (6) 500, (7) 1000, (8) 1500, (9) 2000, and (10) 2500. The radiating antenna is arranged at the catalyst bed outlet.

the convection current of cold gas. In this case, a wave can propagate in the preliminarily heated catalyst bed in the direction of gas filtration. Figure 6 shows the dynamics of temperature changes along the catalyst bed at the radiation intensity $I_0 = 10^6 \text{ cal m}^{-2} \text{ s}^{-1}$, $\chi_\lambda = 0.323$, and $u = 1.2 \text{ m/s}$. As can be seen in Fig. 6, the endothermic reaction front propagates through the preheated catalyst bed in the opposite direction to the gas flow to reach the right boundary of the catalyst bed; then, the process reaches a steady state. In this case, the temperature at the catalyst bed outlet is $T_{\text{out}} = 714.2^\circ\text{C}$ and the conversion is $x_{\text{out}} = 0.8548$. It is obvious that the energy input to the system is insufficient for providing a high conversion. At the gas filtration rate $u = 1.05 \text{ m/s}$, the reaction front moves with a small speed in the opposite direction to the gas flow, whereas at $u = 1.06 \text{ m/s}$ the reaction front moves in the direction of gas filtration with a velocity of about 10^{-5} m/s . Evidently, the rate of gas filtration can be chosen so that the autowave will not move in the laboratory coordinate system; that is, it will be a standing wave [12–14]. This wave is superficially similar to ordinary steady-state conditions because the structure does not move in the laboratory coordinate system. However, in a standing wave, as in a moving wave, all processes (heat and mass transfer, chemical conversion, and heat release) are really compensated in a restricted spatial interval as a whole. Therefore, a standing wave can be accomplished only as a whole. It is impossible to create a part of this structure, for example, as it can be made with a usual steady state, in which the process can be performed at any contact time. The standing-

wave mode is characterized by the fact that it is an unstable regime, and the smallest fluctuations of system parameters can lead to a qualitative change in autowave propagation velocity. The standing autowave can begin to move either in the direction of gas filtra-

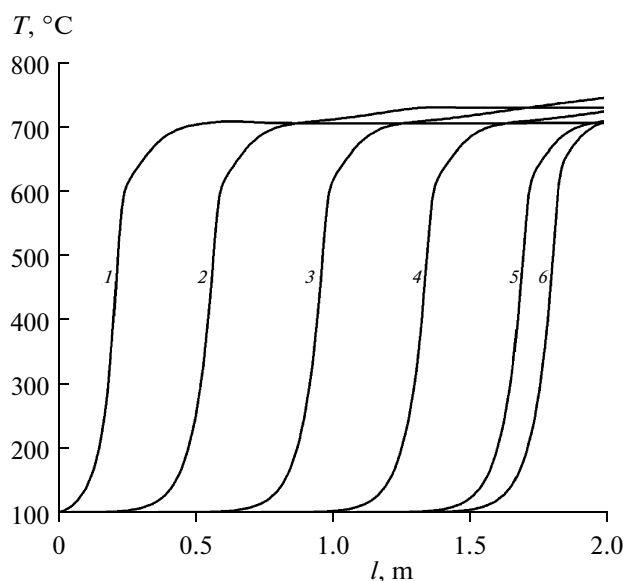


Fig. 6. Dynamics of temperature changes in the catalyst bed at $\chi_\lambda = 0.323$, the radiation intensity $I_0 = 10^6 \text{ cal m}^{-2} \text{ s}^{-1}$, and $u = 1.2 \text{ m/s}$ at different points in time t , s: (1) 100, (2) 500, (3) 1000, (4) 1500, (5) 2000, and (6) 5000. The radiating antenna is arranged at the catalyst bed outlet.

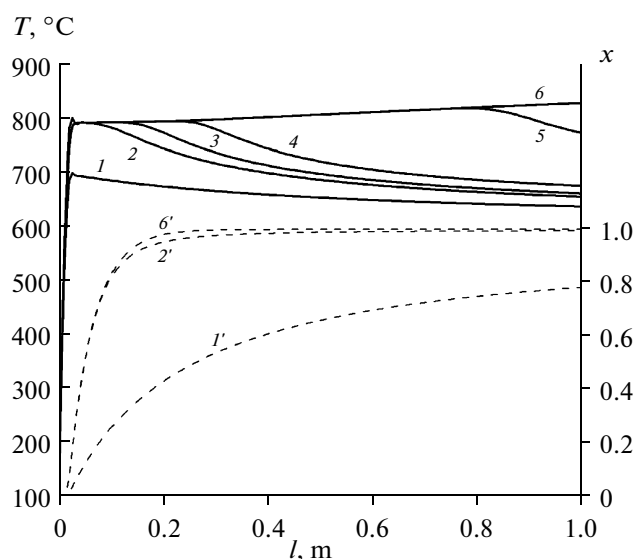


Fig. 7. Dynamics of (solid lines) temperature and (dashed lines) conversion changes in the catalyst bed at $\chi_\lambda = 15$ and the radiation intensity $I_0 = 10^6 \text{ cal m}^{-2} \text{ s}^{-1}$ at different points in time t , s: (1) 10, (2) 20, (3) 50, (4) 100, (5) 500, and (6) 700. The radiating antenna is arranged at the catalyst bed inlet.

tion or in the opposite direction to the gas flow. At the same time, there are simple methods for the stabilization of standing waves.

The mechanism of the appearance and propagation of autowaves by endothermic chemical reaction, which takes place under the action of microwave radiation, is unique. Previously, the autowaves (space-time dissipative structures) of exothermic chemical reactions have been best known and most widely studied [8, 10–14]. The detection and further study of fast autowaves in a catalyst bed in the course of reversible chemical reactions [10–14] led to the understanding of the appearance of space-time dissipative structures with endothermic chemical reaction, which takes place due to the heat accumulated in the catalyst bed. The nature of fast autowaves is such that they can propagate only in the direction of gas filtration, and these space-time dissipative structures can also exist near a thermodynamic equilibrium state [12–14]. The mechanism of the appearance of waves shown in Figs. 5 and 6 is significantly different from the mechanism of fast autowaves. The source of energy (the transformation of microwave energy into thermal energy) in these waves moves in space because the concentration of an absorbing (initial) reactant decreases, and the reaction products are considered optically transparent for microwave radiation. In general, the phenomenon results from the cooperative interaction of linear and nonlinear subsystems—these are the filtration of a cold reaction mixture, the effective thermal conductivity of a catalyst bed, the endothermic chemical

reaction and, and the release of heat due to microwave energy absorption.

The steady-state propagation of autowaves (at a constant velocity and an unchanged spatial structure) is the asymptotic characteristic of a dynamic process, which makes sense only for a catalyst bed of an infinite length at sufficiently long times $t \rightarrow \infty$. Unfortunately, the above results are limited in both space and time. To study the effect of system parameters on the propagation of autowaves, it is reasonable to use the methods and approaches of the theory of combustion: to introduce a moving coordinate system and to go from partial differential equations to ordinary differential equations. This problem will be the subject matter of the future studies.

If the radiating antenna is located at the catalyst bed inlet ($l_s = l$), the formation of a wave is not observed unlike the above case at the same system parameters. Figure 7 shows the dynamics of changes in the temperature and the conversion along the catalyst bed at $\chi_\lambda = 0.323$ and the radiation intensity $I_0 = 10^6 \text{ cal m}^{-2} \text{ s}^{-1}$. As can be seen in Fig. 7, the heating of the reactor occurred most intensely at the inlet of the catalyst bed near the radiating antenna. Approximately 700 s after the onset of the operation of a microwave generator, a steady state is established in the reactor with a sufficiently steep gradient of the inlet temperature; in this case, the temperature and the conversion at the catalyst bed outlet are $T_{\text{out}} = 747.5^\circ\text{C}$ and $x = 0.9990$, respectively.

A cycle of numerical investigations of a quasi-homogeneous model of the fixed bed of a catalyst, in which endothermic chemical reaction occurs with the use of electromagnetic radiation in the microwave range, was performed. The nonlinear law of microwave energy absorption, various versions of the arrangement of a radiation source relative to the direction of gas filtration, and the interaction of microwave radiation with the catalyst and gaseous reactants create various conditions in the reactor for the interaction of internal elementary processes place and, as a result, different steady-state conditions and various dynamics of reaching these steady states. A new phenomenon of the propagation of endothermic chemical reaction autowaves can appear in the case that the catalyst is optically transparent for microwave radiation and one of the initial reactants converts radiant energy into heat.

A number of general regularities in the dynamic behavior of the system and established steady states depending on the values of parameters were determined. The multiparameter system requires the optimization of particular processes conditions; at the same time, the operating practices can be easily controlled. These advantages stimulate the research and development of new technologies in different industries with endothermic chemical reactions that occur under the action of microwave radiation.

Note that the quasi-homogeneous model of the fixed bed of a catalyst is identical to the mathematical description of the filtration combustion of gases when interphase heat exchange is sufficiently intense and a difference between gas and inert solid phase temperatures can be ignored. In this case, all of the above results will also occur in the course of a gas-phase endothermic reaction in an inert granular layer.

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REFERENCES

1. Fedoseev, V.I., Aristov, Yu.I., Tanashev, Yu.Yu., and Parmon, V.N., *Kinet. Catal.*, 1996, vol. 37, no. 6, p. 808.
2. Daminev, R.R., Bikbulatov, I.Kh., Shulaev, N.S., and Rakhmankulov, D.L., *Geterogenno-kataliticheskie promyshlennye protsessy pod deistviem elektromagnitnogo izlucheniya SVCh-diapazona* (Industrial Heterogeneous Catalytic Processes Conducted under the Action of Microwave Radiation), Moscow: Khimiya, 2006.
3. Rakhmankulov, D.L., Bikbulatov, I.Kh., Shulaev, N.S., and Shavshukova, S.Yu., *Mikrovolnovoe izluchenie i intensivatsiya khimicheskikh protsessov* (Microwave Radiation for Intensification of Chemical Processes), Moscow: Khimiya, 2003.
4. Rakhmankulov, D.L., Shavshukova, S.Yu., Daminev, R.R., and Bikbulatov, I.Kh., *Russ. Khim. Zh.*, 2008, vol. 52, no. 4, p. 136.
5. RF Patent 2116826, 1998.
6. Slin'ko, M.G., *Osnovy i printsipy matematicheskogo modelirovaniya kataliticheskikh protsessov* (Fundamentals and Principles of Mathematical Modeling of Catalytic Processes), Novosibirsk: Inst. Kataliza, 2004.
7. Akramov, T.A., Belonosov, V.S., Zelenyak, T.I., Lavrent'ev, M.M., Jr., Slin'ko, M.G., and Sheplev, V.S., *Theor. Found. Chem. Eng.*, 2000, vol. 34, no. 3, p. 263.
8. Kiselev, O.V., Matros, Yu.Sh., and Chumakova, N.A., in *Rasprostraneniye teplovykh voln v geterogennykh sredakh* (Heat Wave Propagation in Heterogeneous Media), Novosibirsk: Nauka, 1988, p. 145.
9. Borekov, G.K., *Geterogennyi kataliz* (Heterogeneous Catalysis), Moscow: Nauka, 1986.
10. Gerashev, A.P., Chumakova, N.A., Matros, Yu.Sh., and Kiselev, O.V., *Teor. Osn. Khim. Tekhnol.*, 1993, vol. 27, no. 2, p. 165.
11. Gerashev, A.P., Chumakova, N.A., and Matros, Yu.Sh., *Chem. Eng. Sci.*, 1997, vol. 52, no. 5, p. 693.
12. Gerashev, A.P., *Russ. J. Phys. Chem.*, 2002, vol. 76, no. 2, p. 161.
13. Gerashev, A.P., *Phys.-Usp.*, 2004, vol. 47, no. 10, p. 991.
14. Gerashev, A.P., *Doctoral (Phys.-Math.) Dissertation*, Novosibirsk: Borekov Inst. of Catalysis, 2010.