Journal of Engineering Physics and Thermophysics, Vol. 80, No. 6, 2007

HEAT- AND MASS TRANSFER IN CHEMICALLY REACTING MEDIA

TURBULENT CONJUGATE HEAT- AND MASS TRANSFER IN CHEMICAL CONVERSIONS IN A TUBULAR REACTOR

L. P. Kholpanov[a] **and Yu. S. Polyakov**[b]

UDC 536.24 (0.63)

A model of turbulent heat- and mass transfer with nonlinear sources (sinks) that appear as a result of chemical reactions of the first and second orders has been developed. The conjugation condition (equality of temperatures and local fluxes) at the reactor — coolant interface was used for this purpose. A finite-difference numerical solution by the alternating direction method is obtained. The influence of the coefficients of turbulent viscosity on heat- and mass transfer is investigated. The model has been tested on the example of modeling fast polymerization processes. It has been established in practical calculations of the processes of fast polymerization that instead of the model with variable coefficients of transfer and velocities of liquid motion one can use its approximation with constant coefficients of transfer and velocities of liquid motion.

Introduction. The processes of turbulent heat- and mass transfer in chemical transformations accompanied by the removal and absorption of heat have found widespread use in thermophysics, chemical technology, and chemical physics [1–4]. The most well-known examples are the processes of combustion and fast polymerization reactions [5, 6].

It appears necessary to allow for heat- and mass transfer in chemical transformations when the characteristic time of a chemical reaction becomes close in value to the characteristic time of heat or substance transfer. The physical processes of substance and heat transfer (diffusion, heat conduction, convection, turbulence, etc., complicated by chemical transformations, especially under the conditions of their turbulent interaction) begin then to exert an appreciable effect on final results, which in the process of solution leads to complex nonlinear mathematical models.

The solutions of these problems are based on the moment of momentum, substance, and energy conservation equations. The solutions themselves are complicated by the presence of small parameters at higher space derivatives and nonlinear sources (sinks). The small parameters at higher derivatives and the great values of sources (sinks) behave differently over different time intervals [1]. All this requires the development of special approaches and methods of solution of heat- and mass transfer problems in chemical transformations.

Of particular interest is modeling of the processes in two-phase flows [7]. It is difficult to adequately describe these processes because one has not only to take into account the equations in the volume of the two-phase space but also to represent correctly the boundary conditions at the phase interface (the surface of phase discontinuity).

In the majority of works, for the description of conjugation at the interface of two phases the well-known Newton law (the boundary condition of the third kind) is used as the boundary condition of the second phase (apart from the equality of substances), whereas the gradient of the substance itself is used for the first phase [5, 8]. A situation arises where the gradient of the substance which characterizes the first phase at the point is equated to the average value of the second phase, which is mathematically incorrect and inadequately represents the physics of the process.

In the present work, as a boundary condition we use the condition of conjugation at the phase interface, viz., the equality of temperatures and of local fluxes. On the one hand, such a statement of the problem complicates the very solution of the problem because of the addition of one other equation of transfer, but, on the other hand, it al-

---

[a] Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, Moscow District, 142432, Russia; email: kholp@icp.ac.ru; [b] "USPolyResearch" Company, Ashland, Pennsylvania, USA. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 80, No. 6, pp. 73–85, November–December, 2007. Original article submitted August 11, 2006.

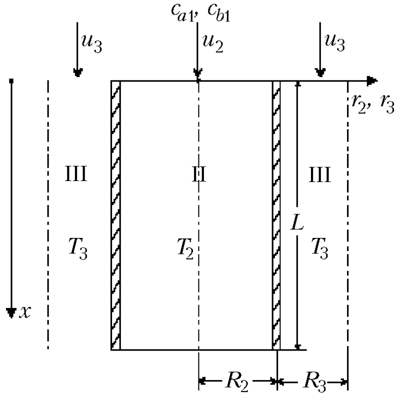

Fig. 1. Schematic of a tubular reactor with cooling from the side of outer wall.

lows one to adequately describe two-phase transfer under the conditions of conjugation at the phase interface. Such a statement of the problem makes it possible to adequately describe the process investigated without resorting to additional experimental data.

Mathematical Model. As an object of investigation we consider turbulent convective heat- and mass transfer in an inner tube (reactor) in which a chemical reaction with liberation (absorption) of heat proceeds (Fig. 1). On the outside the reactor is coaxially cooled (heated) by a turbulent heat carrier flow. At the "reactor–cooling (heating) liquid" phase interface the conjugation conditions — the equality of temperatures and of local heat fluxes — are employed.

Let zone I be composed of the reactor zone and of the coolant (heater) zone; it consists of two concentric tubes (the common zone is not shown in Fig. 1); zone II is the reactor zone, and zone III is the coolant (heater) zone.

A classical example of such a configuration is the process of fast polymerization in a tubular reactor with heat removal through the outer wall [5, 9–12]. It was described with the aid of a nonstationary two-dimensional macrokinetic model that includes the mass conservation laws for the monomer and catalyst and the energy conservation law in the zone of reaction [9]. This problem has been solved numerically for a stationary case at constant (independent of temperature) reaction rates (which corresponds to the occurrence of independent mass- and energy transfer processes), without account for the influence of the cooling liquid temperature distribution on the process of polymerization, and at constant coefficients of turbulent transfer [5].

Below, we mathematically model nonstationary conjugate heat- and mass transfer with allowance for changes in the reaction rates, according to the Arrhenius equation, under the conditions of conjugate statement of the problem, at variable velocity profiles in the reactor and coolant, and with allowance for the distribution of the turbulent transfer coefficients in the reactor. As an example, the proposed model is used to calculate the process of fast polymerization. Despite the fact that the main physicochemical and kinetic data used in our calculations correspond to the processes of fast polymerization, the general model developed by us can be applied to a wide class of problems where there is conjugate turbulent heat- and mass transfer complicated by chemical transformations.

We will consider the case where zone II contains a mixture of two components: *a* (monomer) and *b* (catalyst — an active center), with an exothermal chemical reaction of 2nd order proceeding between them according to the kinetic model of [5]. In this zone, the temperature distribution obeys the laws of convective turbulent heat transfer.

One of the techniques of improving the characteristics of polymers is the removal of heat from reaction zone II, which is accomplished in the zone of the coolant through a thin barrier made from a material of infinite thermal conductivity so that its resistance can be neglected. For this purpose, a cooling liquid is supplied into zone III.

For zone II (the reactor zone), the mathematical model includes the momentum, substance, and energy conservation equations for averaged values of velocity, temperature, and substance:

$$\frac{\partial \mathbf{u}_2}{\partial \tau} + (\mathbf{u}_2 \cdot \nabla)\, \mathbf{u}_2 = \frac{1}{\rho_2} \nabla \cdot \mathbf{P}_2 + \mathbf{F}_2 \,, \tag{1}$$

$$\nabla \cdot \mathbf{u}_2 = 0 \,, \tag{2}$$

$$\frac{\partial c_a}{\partial \tau} + f_1 \frac{\partial^2 c_a}{\partial \tau^2} + (\mathbf{u}_2 \cdot \nabla)\, c_a = \nabla \cdot (\tilde{\mathbf{D}}_2 \cdot \nabla c_a) - k_a c_a c_b \exp\left[-\frac{E_a}{RT_2}\right], \tag{3}$$

$$\frac{\partial c_b}{\partial \tau} + f_2 \frac{\partial^2 c_b}{\partial \tau^2} + (\mathbf{u}_2 \cdot \nabla)\, c_b = \nabla \cdot (\tilde{\mathbf{D}}_2 \cdot \nabla c_b) - k_b c_b \exp\left[-\frac{E_b}{RT_2}\right], \tag{4}$$

$$\rho_2 c_{p2} \left(\frac{\partial T_2}{\partial \tau} + f_3 \frac{\partial^2 T_2}{\partial \tau^2} + (\mathbf{u}_2 \cdot \nabla)\, T_2\right) = \nabla \cdot (\tilde{\lambda}_2 \cdot \nabla T_2) + Q_a k_a c_a c_b \exp\left[-\frac{E_a}{RT_2}\right] \tag{5}$$

and the momentum and energy conservation equations for zone III (the zone of cooling):

$$\frac{\partial \mathbf{u}_3}{\partial \tau} + (\mathbf{u}_3 \cdot \nabla)\, \mathbf{u}_3 = \frac{1}{\rho_3} \nabla \cdot \mathbf{P}_3 + \mathbf{F}_3 , \tag{6}$$

$$\nabla \cdot \mathbf{u}_3 = 0 , \tag{7}$$

$$\rho_3 c_{p3} \left(\frac{\partial T_3}{\partial \tau} + (\mathbf{u}_3 \cdot \nabla)\, T_3\right) = \nabla \cdot (\tilde{\lambda}_3 \cdot \nabla T_3) . \tag{8}$$

For the solution of the system of equations (1)–(8), we will write out the boundary and initial conditions. We introduce the generalized function $F = \{c_a, c_b, T_2\}$. Then, according to the symmetry condition

$$\frac{\partial F}{\partial r_2} = 0 \quad \text{at} \quad r_2 = 0 . \tag{9}$$

The conditions of conjugation of zones II and III are written in the form

$$T_2 = T_3 , \ \ \lambda_2 \frac{\partial T_2}{\partial r_2} = \lambda_3 \frac{\partial T_3}{\partial r_3} \quad \text{at} \quad r_2 = r_3 = R_2 . \tag{10}$$

The conjugation conditions (10) express the equality of temperatures and of local heat fluxes at the interface between zones II and III [1]. Applying them, we can find the local distribution of temperatures in each zone. The conditions of the absence of a flow through the impermeable wall are written in the form

$$\frac{\partial c_a}{\partial r_2} = \frac{\partial c_b}{\partial r_2} = 0 \quad \text{at} \quad r_2 = R_2 . \tag{11}$$

At the boundary of zone III we take the symmetry condition:

$$\frac{\partial T_3}{\partial r_3} = 0 \ \text{at} \ r_3 = R_2 + R_3 . \tag{12}$$

This selection of the boundary condition is based on the assumption that the apparatus in which fast chemical reactions proceed is constructed as a system of tubular elements located in parallel.

We use the condition of the first kind at the inlet to the reactor:

$$c_a = c_{a1}(r_2)\,, \quad c_b = c_{b1}(r_2)\,, \quad T_2 = T_{21}\,, \quad T_3 = T_{31} \quad \text{at} \quad x = 0\,. \tag{13}$$

The condition at the exit is written in the form

$$\frac{\partial F}{\partial x} = 0 \quad \text{at} \quad x = L\,, \quad F = \left\{c_a, c_b, T_2, T_3\right\}. \tag{14}$$

It should be kept in mind that L in Eq. (14) is the length of the reactor. Naturally, the process of heat- and mass transfer can be completed earlier, viz., at a distance from the entrance smaller than the reactor length. In this case, the effective length of heat- and mass transfer can be determined from the condition of attainment of constant values for the concentrations of the monomer and active center (the condition of emergence into a stationary regime). It can also characterize the magnitude of the active section of heat- and mass transfer, the multiplicity of which points to the application of agitators in the case of a slip of the reaction mixture in the reactor.

We will use the initial conditions

$$c_a = c_{a0}\,, \quad c_b = c_{b0}\,, \quad T_2 = T_{20}\,, \quad T_3 = T_{30}\,. \tag{15}$$

Let us simplify the system of equations (1)–(8). We assume that the monomer and catalyst in zone II and the liquid for cooling in zone III move with velocities u_2 and u_3 respectively equal to the distribution of turbulent velocities calculated by one of the models that characterize the law of turbulence attenuation on approach to the wall [13]. The effective coefficients of turbulent transfer can be represented as a sum of turbulent and molecular coefficients, with their values being based on the physical statement of the models which are based on the concept of complete attenuation of turbulent pulsations on the wall. To compare calculations, we also used averaged coefficients of turbulent transfer far from the wall. However, near the wall, at a distance of 2–3 steps from it, it is assumed that these coefficients change by the Landau–Levich law [14]. In both cases it is assumed that the main role near the wall is played by molecular momentum-, substance-, and energy transfer, as is evident, e.g., from conjugation condition (10). We also assume that the convective turbulent transfer depends only on the coordinate in the transverse direction. Since investigations of relaxation and wave processes and of the Monge surface associated with phase transitions or chemical transformations are of independent interest, the influence of these effects on transfer are not taken into account in this work. With these approximations, the system of equations takes the form

equations for zone II

$$\frac{\partial c_a}{\partial \tau} + u_2 \frac{\partial c_a}{\partial x} = \frac{\partial}{\partial x} D_a \frac{\partial c_a}{\partial x} + \frac{1}{r_2} \frac{\partial}{\partial r_2}\left(D_a r_2 \frac{\partial c_a}{\partial r_2}\right) - k_a^0 c_a c_b \exp\left[-\frac{E_a}{RT_2}\right], \tag{16}$$

$$\frac{\partial c_b}{\partial \tau} + u_2 \frac{\partial c_b}{\partial x} = \frac{\partial}{\partial x} D_b \frac{\partial c_b}{\partial x} + \frac{1}{r_2} \frac{\partial}{\partial r_2}\left(D_b r_2 \frac{\partial c_b}{\partial r_2}\right) - k_b^0 c_b \exp\left[-\frac{E_b}{RT_2}\right], \tag{17}$$

$$\rho_2 c_{p2}\left(\frac{\partial T_2}{\partial \tau} + u_2 \frac{\partial T_2}{\partial x}\right) = \frac{\partial}{\partial x} \lambda_2 \frac{\partial T_2}{\partial x} + \frac{1}{r_2} \frac{\partial}{\partial r_2}\left(\lambda_2 r_2 \frac{\partial T_2}{\partial r_2}\right) + Q_a k_a^0 c_a c_b \exp\left[-\frac{E_a}{RT_2}\right]; \tag{18}$$

an equation for zone III

$$\rho_3 c_{p3}\left(\frac{\partial T_3}{\partial \tau} + u_3 \frac{\partial T_3}{\partial x}\right) = \frac{\partial}{\partial x} \lambda_3 \frac{\partial T_3}{\partial x} + \frac{1}{r_3} \frac{\partial}{\partial r_3}\left(\lambda_3 r_3 \frac{\partial T_3}{\partial r_3}\right). \tag{19}$$

The boundary and initial conditions for the solution of the system of equations (16)–(19) are left unchanged.

Calculation of the Turbulent Transfer Coefficients. Since the coefficients of turbulent transfer of substance and energy are related to the coefficient of turbulent viscosity, we must select a model of calculation of the latter. There are different approaches to solving these problems. They are based on various assumptions about the laws of attenuation of turbulent viscosity with approach to the wall. Application of one or another assumptions simplifies the solution of the problem. Otherwise the problem may appear to be within the framework of general statement problems, where almost all of the factors are taken into account but it is difficult to obtain a solution.

In the present work the Boussinesq approximation is used with account for the fact that there is the following relationship between the deviators of the tensors of Reynolds stresses and averaged deformation rates ε_{ij} [13]:

$$\tau_{ij} = 2\mu\chi_n S^n \varepsilon_{ij}\,, \tag{20}$$

where χ_n and n are dimensionless constants; ε_{ij} is the deformation rate tensor which for an incompressible liquid coincides with its deviator. The quantity S represents a positive function of averaged characteristics of turbulent flow; in going from dimensional velocities and coordinates to dimensionless ones it becomes proportional to the Reynolds number. In particular, as shown in [13], this requirement is satisfied by the relations

$$S_1 = \frac{uy}{\nu}\,, \quad S_2 = \frac{u^2}{\nu}\frac{1}{\left|\dfrac{\partial u}{\partial y}\right|}\,, \quad S_3 = \frac{\left|u\dfrac{\partial u}{\partial y}\right|}{\nu\left|\dfrac{\partial^2 u}{\partial y^2}\right|}\,, \quad S_4 = \frac{y^2}{\nu}\left|\frac{\partial u}{\partial y}\right|\,, \quad S_5 = \frac{1}{\nu}\frac{\left|\dfrac{\partial u}{\partial y}\right|^3}{\left|\dfrac{\partial^2 u}{\partial y^2}\right|^2}\,. \tag{21}$$

Equations (20) and (21) allow one to determine the kinematic coefficient of turbulent viscosity. Indeed, from expression (20) it follows that

$$\mu_{\rm t} = \mu\chi_n S^n = \rho\nu_{\rm t}\,, \tag{22}$$

whence

$$\nu_{\rm t} = \nu\chi_n S^n\,. \tag{23}$$

The parameter S entering into the equation for the kinematic coefficient of turbulent viscosity can be determined by one of the relations (21). As is seen from these relations, to find the value of S it is necessary to have the given velocity profile. It can be determined, for example, from the previous layer being included into the general scheme of the calculation algorithm or by the technique suggested in [13]. In the present work the value of S was determined by the technique of [13], according to which the velocity profile is

$$\tilde{u} = \frac{u}{u_0} = \frac{f(n, \eta)}{f(n, 0)} \tag{24}$$

with

$$f(n, \eta) = \int\limits_{\eta}^{1}\left(1 - \eta^{\frac{2n-1}{2n}}\right)^{2n/(1+n)} d\eta\,, \tag{25}$$

where n is the exponent of the quantity S^n in the expression for the kinematic coefficient of turbulent viscosity (23).

Calculations by the turbulence model of [13] were obtained at different values of n, i.e., $n = 2/3$, $3/4$, and $9/10$ in Eq. (23). This choice of the exponents in Eq. (23) is due to the fact that near the tube wall the velocity profiles corresponding to these values asymptotically approach the profiles of turbulence attenuation with approach to the wall by the $1/5$, $1/7$, and $1/19$ power laws. It should be noted that, as mentioned in [13], the variant of the turbulence theory made it possible to adequately describe calculations of all 33 turbulent boundary layers acknowledged by the Stanford conference in 1968 as standard ones.

Using the technique of determining the velocity profile in a turbulent incompressible liquid in a reactor, in particular, by relations (24) and (25), it is possible to reduce the velocity, e.g., at $n = 3/4$ in zone II, to the form

$$\bar{u}_2(\eta) = 1.225\left(1-\eta^{1/3}\right)^{1/7} - 0.306\left(1-\eta^{1/3}\right)^{8/7} + 0.081\left(1-\eta^{1/3}\right)^{15/7}, \tag{26}$$

where

$$u_2 = u_{20}\bar{u}_2(\eta)\,; \quad \eta = r_2/R_2\,. \tag{27}$$

The coefficient of turbulent diffusion for the monomer is then calculated in terms of the number $\mathrm{Sc}_{2\mathrm{t}} = \dfrac{\nu_{2\mathrm{t}}}{D_{a\mathrm{t}}}$ and the value of the kinetic coefficient of turbulent viscosity is determined by Eq. (23) depending on the parameter S^n:

$$\nu_{2\mathrm{t}} = \frac{1}{2}\nu_{2\mathrm{m}}\chi_n \mathrm{Re}_{2\mathrm{m}} G_1(\eta)\,,$$

where, e.g., for $n = 3/4$ the function $G_1(\eta)$ is approximated as

$$\begin{aligned} G_1(\eta) &= -0.25886\eta^4 - 0.59772\eta^3 - 0.84409\eta^2 + 0.50523\eta\,, \quad \eta_{\max} \le \eta \le 1\,; \\ G_1(\eta) &= -0.25886\eta_{\max}^4 - 0.59772\eta_{\max}^3 - 0.84409\eta_{\max}^2 + 0.50523\eta_{\max}, \quad \eta < \eta_{\max}\,. \end{aligned} \tag{28}$$

Here, $\eta_{\max}$ corresponds to the maximum value of the function G_1.

It should be noted that the function $G_1(\eta)$, which uses relations of the type of (21), attains a maximum and tends to zero values on the wall and the axis. We assumed that the zero value of this function on the axis did not correspond to the physical meaning of the change in the kinematic coefficients of turbulent viscosity. This problem was also discussed in [15]; therefore in calculations this dependence was used up to $\eta_{\max}$. Above this value the kinematic coefficient of turbulent viscosity was taken equal to its maximum value. According to these remarks, the effective coefficient of turbulent diffusion, e.g., for the monomer, takes the form

$$D_a = D_{a\mathrm{m}}\left(1 + \frac{D_{a\mathrm{t}}}{D_{a\mathrm{m}}}\right) = D_{a\mathrm{m}}\left(1 + \frac{\chi_n \mathrm{Re}_{2\mathrm{m}}\mathrm{Sc}_{a\mathrm{m}}}{2\mathrm{Sc}_{2\mathrm{t}}} G_1(\eta)\right). \tag{29}$$

Other effective coefficients of turbulent exchange in zones II and III were determined similarly.

Nondimensionalization of the problem. We shall express the basic quantities in terms of dimensionless ones:

$$c_a = c_{a0}\bar{c}_a\,, \quad c_b = c_{b0}\bar{c}_b\,, \quad u_2 = u_{20}\bar{u}_2\,, \quad \tau = tt_0\,, \quad x = \bar{x}x_0\,, \quad r_2 = \bar{r}_2 r_{20}\,. \tag{30}$$

We introduce the "hot" temperature T_*:

$$T_2 = T_* + \theta_2 RT_*^2/E_a\,; \quad \theta_2 = \frac{E_a}{R(T_*)^2}(T_2 - T_*)\,, \quad \beta = RT_*/E_a\,.$$

Then the exponent in the Arrhenius equation can be represented as

$$\exp\left[-\frac{E_a}{RT_2}\right] = \exp\left[-\frac{E_a}{RT_*(1+\theta_2 RT_*/E_a)}\right] = \exp\left[-\frac{1}{\beta(1+\theta_2\beta)}\right] = \exp\left[-\frac{1}{\beta} + \frac{\theta_2}{1+\theta_2\beta}\right].$$

The technique of nondimensionalization of the system of equations (16)–(19) can be illustrated using as an example the energy conservation equation (18). We introduce the following characteristic time of reaction in a volume element (sec·kg/m^3): $\eta_a = 1/(k_a^0 \exp[-1/\beta])$. Then we may use the time scale in the form $t_0 = \eta_a/c_{a0}$.

Using Eq. (18), we determine the scales of x_0 and r_{20}. Having introduced $\lambda_2^* = \lambda_2/(\rho_2 c_{p2})$, $q_a = Q_a/(\rho_2 c_{p2})$, we obtain

$$\frac{\partial T_2}{\partial \tau} + u_2 \frac{\partial T_2}{\partial x} = \frac{\partial}{\partial x} \lambda_2^* \frac{\partial T_2}{\partial x} + \frac{1}{r_2} \frac{\partial}{\partial r_2} \left(\lambda_2^* r_2 \frac{\partial T_2}{\partial r_2} \right) + q_a k_a^0 c_a c_b \exp \left[- \frac{E_a}{R T_2} \right] . \tag{31}$$

This equation yields the estimates of the transverse and longitudinal scales:

$$t_0 = \frac{(x_0)^2}{\lambda_{2\max}^*} , \quad t_0 = \frac{(r_{20})^2}{\lambda_{2\max}^*} , \quad x_0 = \sqrt{\lambda_{2\max}^* t_0} , \quad r_{20} = \sqrt{\lambda_{2\max}^* t_0} ,$$

where $\lambda_{2\max}^* = \max\ (\lambda_2^*)$.

We correct the scale of the longitudinal coordinate with the aid of the parameter $m = x_0/r_{20}$. This allows us to investigate the relationships between the local scale and the scale of the entire reactor. We obtain

$$x_0 = m \sqrt{\lambda_{2\max}^* t_0} , \quad r_{20} = \sqrt{\lambda_{2\max}^* t_0} . \tag{32}$$

Using these scales, we write the system of equations (16)–(19) and boundary conditions in a dimensionless form as

$$\frac{\partial \bar{c}_a}{\partial t} + G_{11} \bar{u}_2 \, (R_{20} \bar{r}_2) \frac{\partial \bar{c}_a}{\partial \bar{x}} = G_{12} d_a \, (\bar{r}_2) \frac{\partial^2 \bar{c}_a}{\partial \bar{x}^2} + \frac{G_{13}}{\bar{r}_2} \frac{\partial}{\partial \bar{r}_2} \left(d_a \, (\bar{r}_2) \, \bar{r}_2 \frac{\partial \bar{c}_a}{\partial \bar{r}_2} \right) - G_{141} \bar{c}_a \bar{c}_b \exp \left[\frac{\theta_2}{1 + \theta_2 \beta} \right] , \tag{33}$$

$$\frac{\partial \bar{c}_b}{\partial t} + G_{41} \bar{u}_2 \, (R_{20} \bar{r}_2) \frac{\partial \bar{c}_b}{\partial \bar{x}} = G_{42} d_b \, (\bar{r}_2) \frac{\partial^2 c_b}{\partial \bar{x}^2} + \frac{G_{43}}{\bar{r}_2} \frac{\partial}{\partial \bar{r}_2} \left(d_b \, (\bar{r}_2) \, \bar{r}_2 \frac{\partial \bar{c}_b}{\partial \bar{r}_2} \right) - G_{441} \bar{c}_b \exp \left[\frac{G_E \theta_2}{1 + \theta_2 \beta} \right] , \tag{34}$$

$$\frac{\partial \theta_2}{\partial t} + G_{21} \bar{u}_2 \, (R_{20} \bar{r}_2) \frac{\partial \theta_2}{\partial \bar{x}} = G_{22} \Lambda_2 \, (\bar{r}_2) \frac{\partial^2 \theta_2}{\partial \bar{x}^2} + \frac{G_{23}}{\bar{r}_2} \frac{\partial}{\partial \bar{r}_2} \left(\Lambda_2 \, (\bar{r}_2) \, \bar{r}_2 \frac{\partial \theta_2}{\partial \bar{r}_2} \right) + G_{241} \bar{c}_a \bar{c}_b \exp \left[\frac{\theta_2}{1 + \theta_2 \beta} \right] , \tag{35}$$

$$\frac{\partial \theta_3}{\partial t} + G_{31} \bar{u}_3 \, [1 - \bar{r}_3 R_{20}] \frac{\partial \theta_3}{\partial x} = G_{32} \Lambda_3 \, (\bar{r}_3) \frac{\partial^2 \theta_3}{\partial \bar{x}^2} + \frac{G_{33}}{\bar{r}_3 + G_{r2}} \frac{\partial}{\partial \bar{r}_3} \left(\Lambda_3 \, (\bar{r}_3) \, (\bar{r}_3 G_{r2}) \frac{\partial \theta_3}{\partial \bar{r}_3} \right) , \tag{36}$$

$$\frac{\partial \bar{c}_a}{\partial \bar{r}_2} = 0 , \quad \frac{\partial \bar{c}_b}{\partial \bar{r}_2} = 0 , \quad \frac{\partial \theta_2}{\partial \bar{r}_2} = 0 \quad \text{for} \quad \bar{r}_2 = 0 , \tag{37}$$

$$\frac{\partial \bar{c}_a}{\partial \bar{r}_2} = 0 , \quad \frac{\partial \bar{c}_b}{\partial \bar{r}_2} = 0 , \quad \theta_2 = \theta_3 , \quad G_2 \frac{\partial \theta_2}{\partial \bar{r}_2} = \frac{\partial \theta_3}{\partial \bar{r}_3} \quad \text{for} \quad \bar{r}_2 = \frac{R_2}{r_{20}} , \quad \bar{r}_3 = 0 , \tag{38}$$

$$\frac{\partial \theta_3}{\partial \bar{r}_3} \quad \text{for} \quad \bar{r}_3 = \frac{R_3}{r_{30}} , \tag{39}$$

$$\bar{c}_a = \bar{c}_{a1} , \quad \bar{c}_b = \bar{c}_{b1} , \quad \theta_2 = \theta_{21} , \quad \theta_3 = \theta_{31} \quad \text{for} \quad x = 0 , \tag{40}$$

$$\frac{\partial \bar{c}_a}{\partial x} = 0\,,\quad \frac{\partial \bar{c}_b}{\partial x} = 0\,,\quad \frac{\partial \theta_2}{\partial x} = 0\,,\quad \frac{\partial \theta_3}{\partial x} = 0 \quad \text{for} \quad \bar{x} = \frac{L}{x_0}\,, \tag{41}$$

$$\bar{c}_a = \bar{c}_b = 1\,,\quad \theta_2 = 0\,,\quad \theta_3 = \theta_{30} \quad \text{for} \quad t = 0\,. \tag{42}$$

Here,

$$R_2 = r_{30} G_{r2}\,,\quad R_{20} = \frac{r_{20}}{R_2}\,,\quad \theta_3 = \frac{T_3 - T_*}{\beta T_*}\,,\quad \theta_{30} = \frac{T_{30} - T_*}{\beta T_*}\,,\quad \theta_{21} = \frac{T_{21} - T_*}{\beta T_*}\,,\quad \theta_{31} = \frac{T_{21} - T_*}{\beta T_*}\,,$$

$$r_3 = \bar{r}_3 r_{30} + R_2\,,$$

$$r_{30} = \frac{R_3 r_{20}}{R_2}\,,\quad G_E = E_b/E_a\,,\quad G_2 = \frac{\lambda_{2\text{m}} R_3}{R_2 \lambda_{3\text{m}}}\,,\quad G_{11} = G_{41} = G_{21} = \frac{u_{20}\sqrt{\eta_a}}{m\sqrt{\lambda^*_{2\max} c_{a0}}}\,,$$

$$G_{12} = \frac{D_{a\max}}{m^2 \lambda^*_{2\max}}\,,\quad G_{42} = \frac{D_{b\max}}{m^2 \lambda^*_{2\max}}\,,\quad G_{13} = \frac{D_{a\max}}{\lambda^*_{2\max}}\,,\quad G_{43} = \frac{D_{b\max}}{\lambda^*_{2\max}}\,,\quad G_{141} = \frac{c_{b0}}{c_{a0}}\,,$$

$$G_{441} = \frac{\eta_a}{\eta_b c_{a0}}\,,\quad G_{22} = \frac{1}{m^2}\,,$$

$$G_{23} = 1\,,\quad G_{241} = \frac{q_a c_{b0}}{\beta T_*}\,,\quad G_{31} = \frac{u_{30}\sqrt{\eta_a}}{m\sqrt{\lambda^*_{2\max} c_{a0}}}\,,\quad G_{32} = \frac{\lambda^*_{3\max}}{m^2 \lambda^*_{2\max}}\,,\quad G_{33} = \frac{\lambda^*_{3\max}}{\lambda^*_{2\max}} \left(\frac{R_2}{R_3}\right)^2\,,$$

$$d_a(\bar{r}_2) = \frac{D_{a\text{m}}}{D_{a\max}} \left(1 + \frac{\chi_n \mathrm{Re}_{2\text{m}} \mathrm{Sc}_{a\text{m}}}{2\mathrm{Sc}_{2\text{t}}} G_1(R_{20}\bar{r}_2)\right),\quad d_b(\bar{r}_2) = \frac{D_{b\text{m}}}{D_{b\max}} \left(1 + \frac{\chi_n \mathrm{Re}_{2\text{m}} \mathrm{Sc}_{b\text{m}}}{2\mathrm{Sc}_{2\text{t}}} G_1(R_{20}\bar{r}_2)\right),$$

$$\Lambda_2(\bar{r}_2) = \frac{\lambda_{2\text{m}}}{\lambda_{2\max}} \left(1 + \frac{\mathrm{Pr}_{2\text{m}} \chi_n \mathrm{Re}_{2\text{m}} G_1(R_{20}\bar{r}_2)}{2\mathrm{Pr}_{2\text{t}}}\right),\quad \Lambda_3(\bar{r}_3) = \frac{\lambda_{3\text{m}}}{\lambda_{3\max}} \left(1 + \frac{\mathrm{Pr}_{3\text{m}} \chi_n \mathrm{Re}_{3\text{m}} G_1[1 - \bar{r}_3 R_{20}]}{2\mathrm{Pr}_{3\text{t}}}\right).$$

Numerical Solution. The system of equations (33)–(36) with boundary and initial conditions (37)–(42) has been solved by the alternating direction method with finite-difference approximations of second order. We will consider the construction of a difference grid on the example of Eq. (33). We omit the bar over the dimensionless coordinates and denote the steps as follows: $h_\tau - t$, $h_i - x$, $h_j - r_2$ or r_3. The step in time h_τ is taken constant and those in h_i and h_j — variable, with $\hbar_i = (h_i + h_{i+1})/2$.

We will approximate the differential terms by the control volume method [16]. The value of the nonlinear term, owing its origin to the chemical reaction, will be taken from the previous step in time. Then for the step $n + 1/2$ (in time)

$$\frac{2}{h_\tau}\left[c_{a,i,j}^{n+1/2} - c_{a,i,j}^{n}\right] + \frac{G_{11}}{2\hbar_i} u_2(R_{20} r_2^j)\left[c_{a,i+1,j}^{n} - c_{a,i-1,j}^{n}\right] = G_{12} d_a(R_{20} r_2^j)\left[\frac{c_{a,i+1,j}^{n}}{\hbar_i h_{i+1}} - \frac{2c_{a,i,j}^{n}}{h_{i+1} h_i} + \frac{c_{a,i-1,j}^{n}}{\hbar_i h_i}\right] +$$

$$+ \frac{G_{13}}{2 r_2^j \hbar_j}\left[d_a\left(\frac{r_2^j + r_2^{j+1}}{2}\right)\left(r_2^j + r_2^{j+1}\right)\frac{c_{a,i,j+1}^{n+1/2} - c_{a,i,j}^{n+1/2}}{h_{j+1}} - d_a\left(\frac{r_2^j + r_2^{j-1}}{2}\right)\left(r_2^j + r_2^{j-1}\right)\frac{c_{a,i,j}^{n+1/2} - c_{a,i,j-1}^{n+1/2}}{h_j}\right] -$$

$$- G_{141} c^{n}_{a,i,j} c^{n}_{b,i,j} \exp\left[\frac{\theta^{n}_{2,i,j}}{1 + \theta^{n}_{2,i,j}\beta}\right],$$

for the step $n + 1$

$$\frac{2}{h_\tau}\left[c^{n+1}_{a,i,j} - c^{n+1/2}_{a,i,j}\right] + \frac{G_{11}}{2\hbar_i} u_2 (R_{20} r_2^{j}) \left[c^{n+1}_{a,i+1,j} - c^{n+1}_{a,i-1,j}\right] = G_{12} d_a (R_{20} r_2^{j}) \left[\frac{c^{n+1}_{a,i+1,j}}{\hbar_i h_{i+1}} - \frac{2c^{n+1}_{a,i,j}}{h_{i+1} h_i} + \frac{c^{n+1}_{a,i-1,j}}{\hbar_i h_i}\right]$$

$$+ \frac{G_{13}}{2 r_2^{j} \hbar_j}\left[d_a \left(\frac{r_2^{j} + r_2^{j+1}}{2}\right)\left(r_2^{j} + r_2^{j+1}\right)\frac{c^{n+1/2}_{a,i,j+1} - c^{n+1/2}_{a,i,j}}{h_{j+1}} - d_a \left(\frac{r_2^{j} + r_2^{j-1}}{2}\right)\left(r_2^{j} + r_2^{j-1}\right)\frac{c^{n+1/2}_{a,i,j} - c^{n+1/2}_{a,i,j-1}}{h_j}\right]$$

$$- G_{141} c^{n}_{a,i,j} c^{n}_{b,i,j} \exp\left[\frac{\theta^{n}_{2,i,j}}{1 + \theta^{n}_{2,i,j}\beta}\right].$$

We will note some specific features appearing in realization of the boundary conditions.

The symmetry condition on the reactor axis leads to the appearance of the indeterminacy of the form of 0/0 in Eqs. (33)–(35). We will resolve this indeterminacy on the example of Eq. (3) for c_a. Indeed, if we represent the second term on the right-hand side of Eq. (33) in the form

$$\frac{G_{13}}{r_2}\frac{\partial}{\partial r_2}\left(d_a (r_2)\, r_2 \frac{\partial c_a}{\partial r_2}\right) = G_{13}\left(\frac{d\,(d_a [r_2]\, r_2)}{dr_2}\frac{1}{r_2}\frac{\partial c_a}{\partial r_2} + d_a [r_2]\frac{\partial^2 c_a}{\partial r_2^2}\right),$$

we obtain the indeterminacy of the form of 0/0 with $\partial c_a/\partial r_2 \to 0$ and $r_2 \to 0$. We resolve the indeterminacy with the aid of the l'Hopital rule:

$$\lim_{r \to 0}\frac{1}{r_2}\frac{\partial c_a}{\partial r_2} = \frac{\partial^2 c_a}{\partial r_2^2}.$$

Then on the axis

$$\frac{d\,(d_a [r_2]\, r_2)}{dr_2}\frac{1}{r_2}\frac{\partial c_a}{\partial r_2} + d_a [r_2]\frac{\partial^2 c_a}{\partial r_2^2} = \left(\frac{d\,(d_a [r_2]\, r_2)}{dr_2} + d_a [r_2]\right)\frac{\partial^2 c_a}{\partial r_2^2}.$$

Substituting this expression into Eq. (33) on the axis $r_2 = 0$, we obtain

$$\frac{\partial c_a}{\partial t} + G_{11} u_2 (R_{20} r_2)\frac{\partial c_a}{\partial x} = G_{12} d_a [r_2]\frac{\partial^2 c_a}{\partial x^2}$$

$$+ G_{13}\left(\frac{d\,(d_a [r_2]\, r_2)}{dr_2} + d_a [r_2]\right)\frac{\partial^2 c_a}{\partial r_2^2} - G_{141} c_a c_b \exp\left[\frac{\theta_2}{1 + \theta_2 \beta}\right],$$

where

$$\frac{\partial^2 c_a}{\partial r_2^2} \approx \frac{c^{n}_{a,i,-2} - 2c^{n}_{a,i,1} + c^{n}_{a,i,2}}{h_1^2} = 2\,\frac{c^{n}_{a,i,2} - c^{n}_{a,i,1}}{h_1^2}.$$

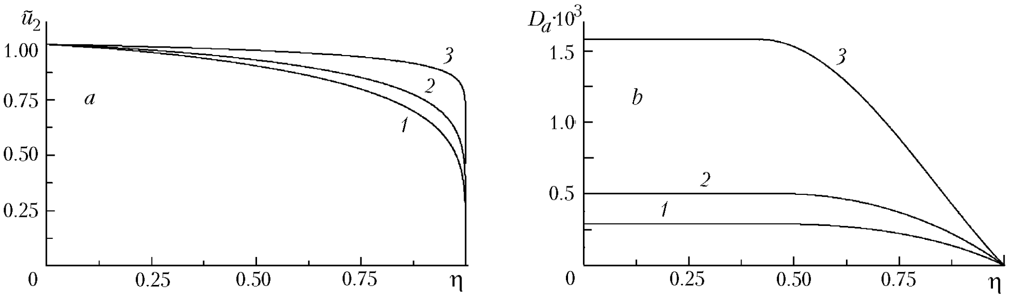

Fig. 2. Dependences of the liquid motion velocity (a) and coefficient of turbulent diffusion (b) on radial coordinate: 1) $n = 2/3$; 2) $3/4$; 3) $9/10$.

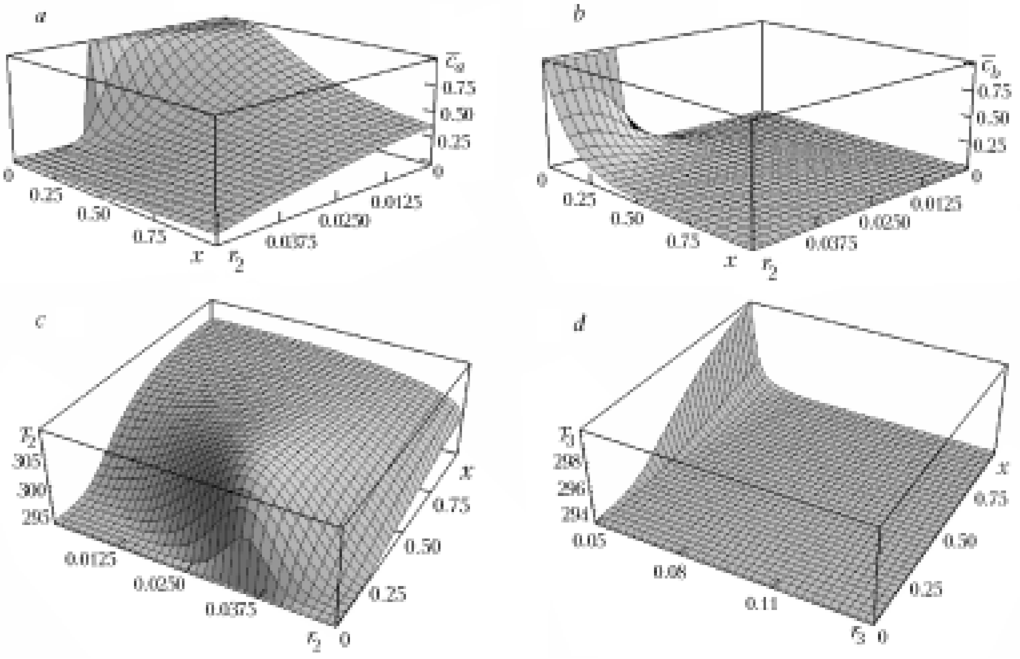

Fig. 3. Dependences of the concentration of the monomer (a), concentration of the active center (b), temperature in the reactor zone (c), and temperature of the cooling liquid (d) on the longitudinal and radial coordinates under stationary conditions for $n = 9/10$.

The solution of the joint system of discretized equations with account for the conjugation conditions on the interface can be obtained in different ways [1]. In the algorithm developed we used a modified pivot method in which, on the reactor axis, the first pivot coefficients are determined. They are "pursued" up to $r_3 = R_2 + R_3$, where the values of the sought-for function by which the entire temperature field is restored are already determined.

In discretization of derivatives in the remaining boundary conditions the Taylor difference approximations with the second-order approximation were used.

Discussion of Results. The calculations were carried out for the process of isobutylene polymerization [5, 17, 18]. Based on the investigations carried out in [5], the following values of computational parameters were selected: $R_2 = 0.05$ m; $R_3 = 0.09$ m; $L = 1$ m; $m = 1$; $\rho_2 = 635$ kg/m^3; $c_{p2} = 2.17 \cdot 10^3$ J/(K·kg); $Q_a = 5.40 \cdot 10^4$ J/mole; $\rho_3 = 1000$ kg/m^3; $c_{p3} = 4.18 \cdot 10^3$ J/(K·kg); $c_{a0} = 10^3$ mole/m^3; $c_{b0} = 2$ mole/m^3; $T_{20} = T_{21} = T_{30} = T_{31} = T_* = 293$ K, $u_{20} = 5$ m/sec; $u_{30} = 7.5$ m/sec; $D_{am} = D_{bm} = 10^{-9}$ m^2/sec; $\lambda_{2m} = \lambda_{3m} = 0.6$ W/(m·K); $\eta_{2m} = \eta_{3m} = 0.5 \cdot 10^{-6}$ Pa·sec; $Sc_{2t} = Pr_{2t} = Pr_{3t} = 1$.

Since there is no reliable technique for estimating reaction rates and effective energies of activation [5, 17, 18], the reaction constants were determined, just as in [5], from the equation

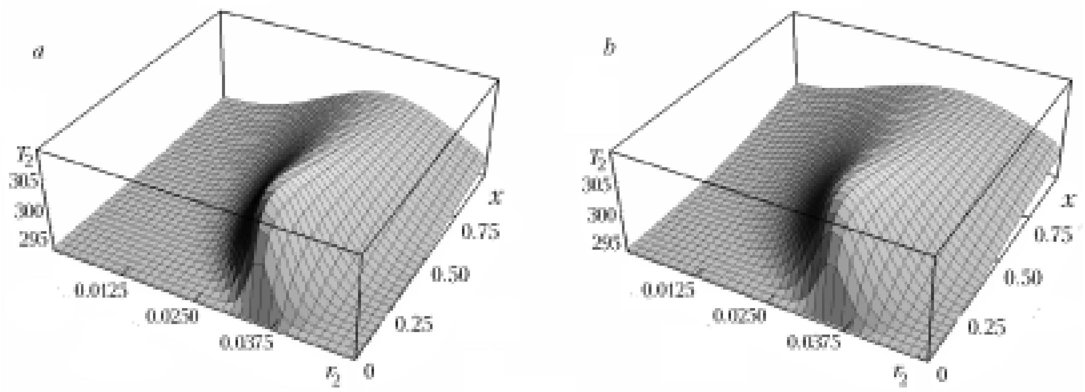

Fig. 4. Dependences of the temperature in the zone of reactor on the longitudinal and radial coordinates under stationary conditions for $n = 2/3$ (a) and $n = 3/4$ (b).

$$\frac{c_a}{c_0} = \exp\left\{-\frac{K_a c_{b1}}{K_b}\left[1 - \exp\left(-\frac{K_b L}{u_2}\right)\right]\right\},$$

which approximately describes the change in the monomer concentration in the absence of radial gradients and with a negligible influence of diffusion in the longitudinal direction. With allowance for [5], the following values were obtained and used in calculations: $k_a = 2.95 \cdot 10^4$ m^3/(mole·sec); $E_a = 1.26 \cdot 10^4$ J/mole; $k_b = 3.37 \cdot 10^4$ sec^{-1}, and $E_b = 1.67 \cdot 10^4$ J/mole.

With the monomer and catalyst being supplied separately, the boundary conditions for concentrations at the entrance were prescribed in the form

$$\frac{c_a}{c_0} = \exp\left\{-\frac{K_a c_{b1}}{K_b}\left[1 - \exp\left(-\frac{K_b L}{u_2}\right)\right]\right\},$$

where U is the Heaviside function, $k \in (0, 1)$.

In the present work, the calculations were made at $k = 0.7$, which corresponds to the condition of the supply of the catalyst into the "ring" from R_2 to $0.7R_2$ (near the reactor wall) and of the monomer — into the central region of the reactor limited by the radius $0.7R_2$.

The discretization steps h_1 and h_j were assumed constant.

The dependences of the velocity of liquid motion and of the diffusion coefficient on the radial coordinate for three values of n are presented in Fig. 2. The higher n, the larger the section in which the velocity takes values close to a maximum. Moreover, the diffusion coefficient attains the highest value at $n = 9/10$. Since this value, approximately equal to $1.5 \cdot 10^{-3}$ m^2/sec, agrees well with the well-known experimental data for a turbulent tube flow [15], the main body of calculations was made at $n = 9/10$.

The distributions of the concentration and temperature fields of the monomer and catalyst in the reactor (in zone II) and of the cooling liquid temperature in zone III are presented in Fig. 3. As follows from Fig. 3a and b, a sharp fall in the monomer and catalyst concentration is observed at the entrance of the reactor; its front is gradually displaced to the side of the reactor symmetry axis. The rate of change in the concentrations of reagents and catalyst decreases gradually from the side of the reactor wall, where the reaction products are cooled by the liquid of zone III. Here, as is seen from Fig. 3c and d, the process of heat release in the volume of the reactor due to chemical reactions and the subsequent cooling of the reaction product are presented in this figure as two competing processes. Moreover, the dependence of temperature in the reaction zone (see Fig. 3c) attains a maximum. The situation is optimal when the reaction heat is immediately removed by the cooling liquid. As the distance from the reactor entrance increases, the steepness of the peak is gradually blurred, indicating the enhancement of the influence of diffusion processes.

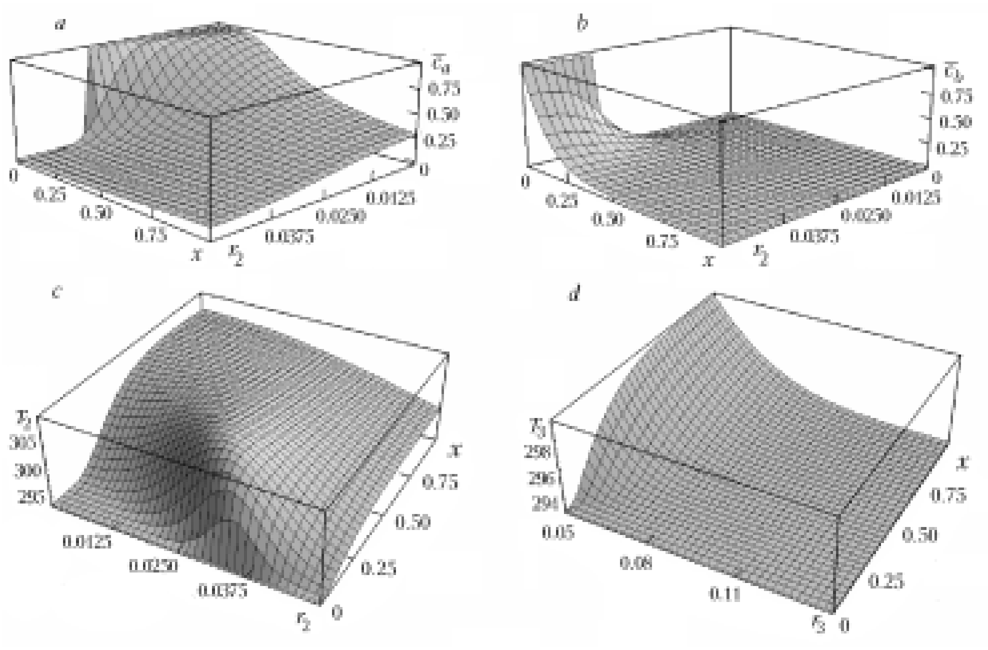

Fig. 5. Dependences of the concentration of the monomer (a), concentration of the active center (b), temperature in the zone of reactor (c), and of the temperature of the cooling liquid (d) on the longitudinal and radial coordinates under stationary conditions in the case of constant values of the coefficients of transfer and liquid flow velocity.

The temperature distributions in the reactor for $n = 2/3$ and $3/4$ are presented in Fig. 4. It is seen that at $n = 2/3$ the temperature peak is virtually localized, since the heat and substance transfer velocity takes minimum values in this case. On the other hand, at $n = 9/10$ (Fig. 3c) the temperature profile at the exit from the reactor is virtually uniform. The value $n = 3/4$ corresponds to an intermediate case. In actual fact, different values of n correspond to different rates of mixing. The higher the rate, the closer the temperature profile to the uniform one.

The concentration and temperature fields were calculated also for the case where the coefficients of transfer and liquid flow velocities were taken constant (Fig. 5). As the constant values of the transfer coefficients we used maximum values of these coefficients, calculated by the model for $n = 9/10$. It is seen that the concentration and temperature profiles in the reactor zone virtually coincide with the corresponding profiles in Fig. 3. Only the temperature field in the zone of the cooling liquid differs strongly in the cases of constant and variable coefficients of transfer. The same results were obtained for $n = 2/3$ and $3/4$.

Conclusions. In practical calculations it is possible to use a model with constant coefficients of transfer and liquid motion velocities. In particular, such a model can be used to determine the diffusion coefficients (rates of the supply of reagents), which make it possible to attain the needed efficiency of the polymerization processes and other processes of conjugate heat and mass transfer in chemical transformations.

NOTATION

c, concentration, mole/m^3; c_p, heat capacity, J/(K·kg); $\tilde{\mathbf{D}}$, diffusion tensor; $D_{j\mathrm{t}}$, $D_{j\mathrm{m}}$, $j = a, b$, coefficients of turbulent and molecular diffusion, m^2/sec; d, dimensionless coefficient of turbulent diffusion; E_a, effective activation energy of monomer reaction with an active center (of chain growth), J; E_b, effective activation energy of the reaction of the breaking of circuit, J; $\mathbf{F}$, vector of volumetric forces; f_1, f_2, f_3, parameters of hyperbolic-type equation, sec; G_1, function of the dependence of the coefficient of turbulent viscosity on radial coordinate; h_j, step of discretization in the radial direction; h_i, step of discretization in the longitudinal direction; h_τ, step of discretization in time; K_a, specific rate of the reaction of the monomer with an active center (increase in circuit), m^3/(mole·sec); K_b, specific rate of reaction of circuit breaking, 1/sec; k, parameter responsible for separate entry of the monomer and catalyst solutions; k_a, pre-exponential multiplier of the rate of monomer reaction with an active center (growth of the chain), $m^3/(mole \cdot sec)$; k_b, pre-exponential multiplier of the rate of reaction of chain breaking, 1/sec; L, length of reactor, m; Pr, Prandtl number; $\mathbf{P}$, tensor of surface forces; Q_a, heat of reactor of a monomer with an active center (growth of chain), J/mole; $\mathrm{Re} = 2u_{i0}R_i/\nu_i$, $i = 2, 3$, Reynolds number; R, universal gas constant, J/K; R_2, radius of a tubular reactor, m; R_3, "radius" of the cooling zone, m; r_2, radial coordinate in zone II, m; r_3, radial coordinate in zone III, m; r_{20}, nondimensionalization scale for r_2, m; r_{30}, dimensionalization scale for r_3, m; $\bar{r}_2$, dimensionless radial coordinate in zone II; $\bar{r}_3$, dimensionless radial coordinate in zone III; $\mathrm{Sc}_{2t} = \nu_{2t}/D_{at}$, turbulent Sherwood number; Sc_{am}, molecular Sherwood number; S, "local Reynolds number" [13]; T, temperature, K; T_*, characteristic temperature in the transformed Arrhenius equation, K; t, dimensionless time; $\mathbf{u}$, velocity vector; u, averaged value of velocity, m/sec; x, longitudinal coordinate, m; $\bar{x}$, dimensionless longitudinal coordinate; y, transverse coordinate, m; $\beta = RT_*/E_a$, dimensionless parameter; ε_{ij}, deformation rate tensor, 1/sec; $\eta = r_2/R_2$, dimensionless radial coordinate in Eq. (26); η_a, characteristic time of reaction of monomer with active center, sec; η_b, characteristic time of reaction of chain breaking, sec; θ, dimensionless temperature; Λ, dimensionless coefficient of turbulent thermal conductivity; $\tilde{\lambda}$, thermal conductivity tensor; λ, coefficient of molecular thermal conductivity, $J/(K \cdot m \cdot sec)$; λ^*, reduced coefficient of turbulent thermal conductivity, m^2/sec; $\mu = \nu\rho$, dynamic coefficient of liquid viscosity, Pa·sec; ν_t and ν, kinematic coefficients of turbulent and molecular viscosity; ρ, density, kg/m^3; τ, time, sec; χ, constant. Subscripts and superscripts: 0, initial value; 1, value at the reactor entrance; 2, zone II; 3, zone III; a, monomer; b, catalyst (active center); m, molecular; max, maximum value of G_1; t, turbulent.

REFERENCES

1. L. P. Kholpanov and V. Ya. Shkadov, *Hydrodynamics and Heat and Mass Exchange with an Interface* [in Russian], Nauka, Moscow (1990).
2. D. A. Frank-Kamenetskii, *Diffusion and Heat Conduction in Chemical Kinetics* [in Russian], Nauka, Moscow (1987).
3. A. I. Vol'pert and S. I. Khudyaev, *Analysis in the Class of Discontinuous Functions and the Equations of Mathematical Physics* [in Russian], Nauka, Moscow (1975).
4. *Proceedings of the 2nd Russian National Conference on Heat Transfer*, in 8 vols., Vol. 3, *Free Convection. Heat Transfer in Chemical Conversions* [in Russian], MEI, Moscow (1998).
5. K. S. Minsker and A. A. Berlin, *Fast Polymerization Processes*, Gordon & Breach, Amsterdam (1996).
6. P. E. Matkovskii, S. M. Aldoshin, V. N. Troitskii, G. P. Startseva, et al., *Development and Industrial Implementation of the Process of Obtaining Synthetic Oligodecene Oils* [in Russian], IPKhF RAN, Chernogolovka (2004).
7. Academician S. S. Kutateladze, *Selected Papers* [in Russian], Nauka, Novosibirsk (1989).
8. A. A. Samarskii and P. N. Vabishchevich, *Computational Heat Transfer* [in Russian], Editorial URSS, Moscow (2003).
9. A. A. Berlin, K. S. Minsker, Yu. A. Sangalov, et al., Calculation and simulation of the polymerization of isobutylene as a fast reaction, *Polym. Sci. USSR*, **22**, 625–634 (1981).
10. A. A. Berlin, Yu. A. Minsker, Yu. A. Prochukhan, and N. S. Enikolopyan, Macroscopic kinetics of fast polymerization processes, *Vysokomol. Soedin.*, **31** (A), No. 9, 1779–1798 (1989).
11. K. S. Minsker, V. P. Zakharov, and A. A. Berlin, Plug-flow tubular turbulent reactors: A new type of industrial apparatus, *Theor. Found. Chem. Eng.*, **35**, No. 2, 162–167 (2001).
12. K. S. Minsker, A. A. Berlin, V. P. Zakharov, et al., Fast reactions in polymer synthesis, *Russ. J. Appl. Chem.*, **76**, No. 2, 264–270 (2003).
13. V. V. Novozhilov, *Theory of a Plane Turbulent Boundary Layer of an Incompressible Liquid* [in Russian], Sudostroenie, Leningrad (1977).
14. V. G. Levich, *Physicochemical Hydrodynamics* [in Russian], Fizmatlit, Moscow (1959).
15. B. S. Petukhov, *Problems of Heat Transfer. Selected Papers* [in Russian], Nauka, Moscow (1987).
16. P. J. Roache, *Computational Fluid Dynamics* [Russian translation], Mir, Moscow (1980).

17. J. P. Kennedy, A. Shinkawa, and F. J. Williams, Fundamental studies on cationic polymerizations: molecular weights and molecular weight distributions of polyisobutylenes produced by γ-irradiation (free ions) and chemical catalysis (ion pairs), *Polym. Sci. A-1*, **9**, No. 6, 1551–1561 (1971).
18. R. B. Taylor and F. Williams, Kinetics of ionic processes in the radiolysis of liquids. V. Cationic polymerization of isobutylene under anhydrous conditions, *J. Am. Chem. Soc.*, **91**, No. 14, 3728–3732 (1969).