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ON STATIONARY CONDITIONS OF WORK OF CHEMICAL REACTORS WITH LONGITUDINAL AND TRANSVERSE MIXING*

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A two-dimensional model of chemical reactor is proposed and investigated. The model generalizes the model of ideal displacement with integral allowance for heat emission /1/ on the case when in the reactor the radial temperature gradient is substantial. For the proposed model the existence of at least one stationary solution is proved for any parameters of the system. The sufficient criteria are determined for the existence of a stationary mode in the region of parameter variation in which this mode is unique. Comparison with the respective mode /1/ show that outside the neighborhood of the boundary of regions of parameters with various numbers of modes, the stationary solutions for the proposed model are a regular perturbations of solutions /1/. An asymptotic expansion of solutions is constructed for small Péclet numbers and an approximate solution is given for moderate Péclet numbers, based on a quadratic approximation of the radial temperature profile is given. Obtained results are supported by numerical calculations, which use the finite-difference approximation of initial differential equations and the methods of ranging /2/ or local variation /3/ for solving the two-point respective boundary value problem.

For the described processes of heat and mass transfer in a flowing chemical reactor and reactors with suspended layer generally are used one-dimensional models supplemented by simplifying assumptions about the transport processes (perfect displacement or total intermixing). The existence, uniqueness, and the stability of steady modes of such reactors was the subject of fairly large attention /4-6/. However, for a number of heterogeneous catalytic processes that occur with considerable heat release, the transverse temperature gradient becomes important, necessitating the introduction in the consideration the mechanism of transverse thermal conductivity and heat transfer on the wall to the heat carrier.

The domain of application of the proposed here two-dimensional model may be the description of high egzothermal processes in fluidized beds, where the reagents motion is close to the mode of ideal displacement, and the values of effective thermal conductivity coefficients are large owing to the intensive motion of the catalyst particles. This model may also be used for the analysis the conditions of reactor operation with a stationary layer of the catalyst, in which the value of the effective thermal conductivity coefficient in the transverse direction is considerably lower than in the longitudinal /7,8/.

1. The reactor model. The two-dimensional model of chemical reactor of ideal displacement with respect to the matter (the longitudinal and transverse diffusion coefficients are zero) and complete longitudinal intermixing with respect to energy (the longitudinal thermal conductivity coefficient is infinite, while the transverse is finite). For simplicity it is assumed that the velocity profile is plane and the chemical reaction is of first order, although the basic conclusions are valid for reactions of any order.

The stationary equations of mass and heat transfer for the considered model of reactor are in the dimensionless form as follows:

$$\frac{\partial\xi}{\partial x}-g\exp\left(-\frac{\beta}{\theta}\right)(1-\xi)=0 \tag{1.1}$$

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{d\theta}{dr}\right)=\mathrm{Pe}\left[\theta-\theta''-g\exp\left(-\frac{\beta}{\theta}\right)\int_0^1(1-\xi)\,dx\right] \tag{1.2}$$

$$\xi=\frac{C^\circ-C}{C^\circ},\quad \theta=\frac{T}{T_*},\quad \theta''=\frac{T''}{T_*},\quad T_*=\frac{hC^\circ}{\rho c},\quad g=\frac{k_0l}{u}$$

$$\beta=\frac{E}{R_0T_*},\quad \mathrm{Pe}=\frac{\varepsilon_0\rho ca^2u}{\lambda l},\quad x=\frac{X}{l},\quad r=\frac{R}{a}$$

where C and C° is the concentration of the key substance in the reactor and at entry into the

*Prikl.Matem.Mekhan.,Vol.47,No.1,pp.73-81,1983 latter, respectively, T and T'' are the temperatures respectively of the reactor and the temperature of the entering mixture, h is the heat of reaction, ρ and c are the density and the specific heat of the mixture of reagents and the product of reaction, E is the activation energy, R_0 is the gas constant, k_0 is the Arrenhius preexponent, u is the mixture velocity, l and a are the length and radius of the reactor, X and R are the longitudinal $(0 \leqslant X \leqslant l)$ and transverse $(0 \leqslant R \leqslant a)$ coordinates, ε_0 is the volume part of the mixture of reagents and of product of reaction in the porous layer of catalyst, λ is effective value of the coefficient of the thermal conductivity in the radial direction, and g is a parameter proportional to the Damkeller number.

Equations (1.1) and (1.2) are supplemented by the boundary conditions

$$x = 0, \quad \xi = 0 \tag{1.3}$$

$$r = 0, \quad d\theta/dr = 0 \tag{1.4}$$

$$r = 1, \quad d\theta/dr + \mathrm{Bi}\,(\theta - \theta') = 0$$

$$\theta' = \frac{T'}{T_*}, \quad \mathrm{Bi} = \nu\,\mathrm{Pe}, \quad \nu = \frac{\alpha l}{\varepsilon_0 \rho c a u}$$

where Bi is the Biot number, T' is the temperature of the heat carrier, and α, is the coefficient of heat transfer by the heat carrier through the wall.

Since the effective coefficients of transfer for the substance and heat in the considered here model of reactor substantially differ, it is interesting to estimate the characteristic dimensions of the reactor, for which such model is acceptable. The characteristic time of diffusion processes transfer of the substance $\tau_D = \min(a^2/D_r, l^2/D_x)$ (where D_r, D_x are the effective coefficients of diffusion in the transverse and longitudinal directions, respectively) significantly greater than the time of its transfer by the stream along the reactor $\tau_u = l/u$. The characteristic time of transmission of heat by thermal conductivity in the longitudinal direction $\tau = l^2/\chi_x$ is, on the contrary, by far smaller of time τ_u, and the characteristic time of transfer of heat in the transverse direction $\tau_r = a^2/\chi_r$ is comparable with τ_u (here χ_x, χ_r are the effective coefficients if thermal conductivity in the longitudinal and transverse directions, respectively; $\chi = \lambda/(\rho c)$). Then the reactor dimensions must satisfy the following requirements:

$$\chi_x/u > l > D_x/u, \quad \sqrt{\chi_r \chi_x}/u > a > \sqrt{D_r D_x}/u$$

The stationary distribution of the degree of reaction advancement is determined by the solution of Eq. (1.1) with the boundary condition (1.3) and is connected to the temperature radial distribution by the relation

$$\xi(x, r) = 1 - \exp(-xg \exp(-\beta/\theta(r))) \tag{1.5}$$

Substituting (1.5) into (1.2), we obtain for the determination of stationary distribution of temperature along the reactor radius the equation

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{d\theta}{dr}\right) = \mathrm{Pe}\,F(\theta); \quad F(\theta) = \theta - \theta'' - 1 + \exp\left(-g\exp\left(-\frac{\beta}{\theta}\right)\right) \tag{1.6}$$

The number of solutions of the two-point boundary value problem (1.6), (1.4) determines the number of stationary modes of reactor operation. By virtue of nonlinearity of function $F(\theta)$ there can be several stationary modes.

2. On the existence of solution. The two-point boundary value problem (1.4), (1.6) has at point $r = 0$ a nonsummable singularity. But by virtue of boundedness of function $F(\theta)$ it is possible to solve the problem of its existence. In this case it is possible to take advantage of the theorem /9/ in conformity with which the solution of two-point boundary value problem with a nonsummable singularity does exist, if there exist an upper $(\alpha'(r))$ and a lower $(\alpha(r))$ functions of the problem that satisfy specific conditions and $\alpha'(r) \geqslant \alpha(r)$. The solution lies between the upper and lower functions

$$\alpha(r) \leqslant \theta(r) \leqslant \alpha'(r) \tag{2.1}$$

Such functions for problem (1.4), (1.6) can be constructed

$$\alpha'(r) = \theta'' + 1 + I(\mathrm{Pe})(\theta' - \theta'' - 1)\, I_0(r\sqrt{\mathrm{Pe}}) \tag{2.2}$$

$$\alpha(r) = \theta'' + I(\mathrm{Pe})(\theta' - \theta'')\, I_0(r\sqrt{\mathrm{Pe}})$$

$$I(\mathrm{Pe}) = \mathrm{Bi}\,[I_1(\sqrt{\mathrm{Pe}})\sqrt{\mathrm{Pe}} + \mathrm{Bi}\, I_0(\sqrt{\mathrm{Pe}})]^{-1} > 0$$

where I_0 and I_1 are modified Bessel functions of zero and first order.

It can be shown that the estimate (2.1), (2.2) remains valid for all solutions of problem

(1.4), (1.6), when there are several of them. Condition (2.1) in the limit case $\mathrm{Pe} = 0$ (heat propagates along the radius considerable quicker than it is carried away by the stream along the reactor) reduces to the following:

$$\frac{\mathrm{Pe}\,\theta'' + 2\,\mathrm{Bi}\,\theta'}{\mathrm{Pe} + 2\,\mathrm{Bi}} \leqslant \theta \leqslant \frac{\mathrm{Pe}\,(1 + \theta'') + 2\,\mathrm{Bi}\,\theta'}{\mathrm{Pe} + 2\,\mathrm{Bi}}$$

and in the opposite case $(\mathrm{Pe} \to \infty)$

$$\theta'' + (\theta' - \theta'')\exp\left(-\sqrt{\mathrm{Pe}}\,(1 - r)\right)/\sqrt{r} \leqslant \theta(r) \leqslant \theta'' + 1 + (\theta' - \theta'' - 1)\exp\left(-\sqrt{\mathrm{Pe}}\,(1 - r)\right)/\sqrt{r}$$

3. Sufficient conditions of uniqueness. For simpler models considered earlier the possibility of existence of several stationary modes of chemical reactors operation was demonstrated. It is therefore expected that in the considered here case the solution will be generally nonunique.

For the determination of the sufficient condition of uniqueness of solution of problem (1.4), (1.6) we consider the difference of two solutions $\Delta\theta(r) = \theta_2(r) - \theta_1(r)$ that satisfy the equations

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{d\Delta\theta}{dr}\right) = \mathrm{Pe}\,[F(\theta_2) - F(\theta_1)] \tag{3.1}$$
$$r = 0,\ d\theta/dr = 0;\ r = 1,\ d\theta/dr + \mathrm{Bi}\,(\theta - \theta') = 0$$

Using the Green's function

$$G(r, t;\ \mathrm{Bi}) = \begin{cases} 1/\mathrm{Bi} - \ln(r), & t \leqslant r \\ 1/\mathrm{Bi} - \ln(t), & t > r \end{cases}$$

problem (3.1) reduces to the integral equation

$$\Delta\theta = -\,\mathrm{Pe}\int_0^1 G(r, t;\ \mathrm{Bi})\,[F(\theta_2) - F(\theta_1)]\,t\,dt \tag{3.2}$$

Owing to the boundedness of function $F(\theta)$ it satisfies the Lipschitz condition with constant M

$$M \leqslant 1 + g^*/\beta,\quad g^* = (\ln g + 2/\ln g)^2/e \tag{3.3}$$

Then from (3.2) we have

$$\left[1 - \mathrm{Pe}\left(\frac{1}{4} + \frac{1}{2\,\mathrm{Bi}}\right)M\right]\max_r |\Delta\theta| \leqslant 0$$

It follows from here that solution is unique $(\Delta\theta \equiv 0)$, if

$$\mathrm{Pe}\left(\frac{1}{4} + \frac{1}{2\,\mathrm{Bi}}\right)M < 1 \tag{3.4}$$

With increasing Péclet number the region in which the solution is necessarily unique, narrows. One more criterion of uniqueness can be established, which provides a weaker estimate of the region of uniqueness at high Péclet numbers. For this we separate in the right-hand side of Eq. (1.6) the component proportional to $\Delta\theta$ and write problem (3.1) in the form

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{d\Delta\theta}{dr}\right) - \mathrm{Pe}\,\Delta\theta = \mathrm{Pe}\,[\varphi(\theta_2) - \varphi(\theta_1)] \tag{3.5}$$
$$\varphi(\theta) = \exp\left(-g\exp\left(-\frac{\beta}{\theta}\right)\right)$$
$$r = 0,\ d\Delta\theta/dr = 0;\ r = 1,\ d\Delta\theta/dr + \mathrm{Bi}\,\Delta\theta = 0$$

For this problem the sufficient condition of uniqueness, similar to (3.4), is

$$\mathrm{Pe}\max_r\left|\int_0^1 G^*(r, t;\ \mathrm{Bi})\,t\,dt\right| m < 1 \tag{3.6}$$

where m is the Lipschitz constant $\varphi(\theta)$ $(m = M - 1)$, and G^* is the Green's function of problem (3.5). From the definition of Green's function follows

$$\int_0^1 G^*(r, t; \mathrm{Bi})\, t\, dt = \Delta\theta|_{\mathrm{Pe}(\varphi_2-\varphi_1)=-1}$$

The solution of problem (3.5) with right-hand side $\mathrm{Pe}(\varphi_2 - \varphi_1) = -1$ is known

$$\Delta\theta|_{\mathrm{Pe}(\varphi_2-\varphi_1)=-1} = \frac{1}{\mathrm{Pe}}\left[1 - I(\mathrm{Pe})\, I_0(r\sqrt{\mathrm{Pe}})\right]$$

(function $I(\mathrm{Pe})$ was determined earlier in (2.2)). We then have

$$\max_r \left|\int_0^1 G^*(r, t; \mathrm{Bi})\, t\, dt\right| = \frac{1}{\mathrm{Pe}}\left[1 - I(\mathrm{Pe})\right]$$

and the sufficient condition of uniqueness of (3.6) assumes the form

$$[1 - I(\mathrm{Pe})]\, m < 1 \tag{3.7}$$

Note that condition (3.7) is a generalization of Van Hirden /6/ for the problem considered here. In the limit case $\mathrm{Pe} \to 0$ (reactor of total intermixing with respect to temperature) it reduces to

$$m < 1 + 2\nu, \quad \nu = \mathrm{Bi}/\mathrm{Pe} \tag{3.8}$$

and has the simple physical meaning: the maximum slope of heat release curve is smaller slope than that of heat transfer curve.

A weaker but simpler criterion of uniqueness can be obtained from (3.7), using the upper limit of Lipschitz's constant m. According to (3.3) $m = M - 1 < g^*/\beta$. Then (3.7) is reduced to the condition

$$\beta > g^*[1 - I(\mathrm{Pe})] \tag{3.9}$$

and in the limit case of $\mathrm{Pe} \to 0$ assumes a particularly simple form

$$\beta(1 + 2\nu) > g^* \tag{3.10}$$

Note that one more, the weaker, but uniform over Pe condition of uniqueness is implied by (3.9), if one takes into account that $I(\mathrm{Pe})$ is always greater than zero

$$\beta > g^* \tag{3.11}$$

Conditions (3.9)– (3.11) define the domain of variation of parameter β for which the stationary mode is unique.

A similar condition can be found for the temperature of the heat carrier θ' and the temperature at entry θ'' using the estimate of solution (2.1) by means of the upper and lower functions. Since

$$m = \max_z \left|\frac{1}{\beta} gz \exp(-gz) \ln z\right|, \quad z = \exp\left(-\frac{\beta}{\theta}\right)$$

and $gz\exp(-gz) < e$, the sufficiency condition of uniqueness (3.7) reduces to the following:

$$\min_r \theta > [\beta(1 - I(\mathrm{Pe}))/e]^{1/2}$$

It is reduced to the form (using the estimate (2.1))

$$\theta'' + (\theta' - \theta'')\, I(\mathrm{Pe})\, \eta(\sqrt{\mathrm{Pe}}) > [\beta(1 - I(\mathrm{Pe}))/e]^{1/2} \tag{3.12}$$

$$\eta(\sqrt{\mathrm{Pe}}) = \begin{cases} I_0(\sqrt{\mathrm{Pe}}), & \theta'' \geqslant \theta' \\ 1, & \theta'' < \theta' \end{cases}$$

and in the limit cases has the simple form

$$\theta'' + 2\nu\theta' > [\beta(1 + 2\nu)/e]^{1/2}, \quad \mathrm{Pe} \to 0 \tag{3.13}$$

$$\min_r (\theta'', \theta') > (\beta/e)^{1/2}(1 + \nu^{-1}/\sqrt{\mathrm{Pe}}), \quad \mathrm{Pe} \to \infty$$

4. The asymptotic expansion of solution for small Péclet number. The solution of problem (1.2), (1.4) can be obtained by the method of small parameter when $\mathrm{Pe} \ll 1$, which corresponds to the case when heat propagates along the radius considerably more rapidly than is carried away by the stream along the reactor.

We seek the temperature distribution in the reactor, in the form

$$\theta = \theta_0 + \mathrm{Pe}\,\theta_1 + \mathrm{Pe}^2\theta_2 + \ldots \tag{4.1}$$

Substituting expansion (4.1) into Eq.(1.2) and boundary conditions (1.4), we obtain a sequence of linear problems for the determination of functions θ_i $(i = 0, 1, 2, \ldots)$

$$\begin{aligned} &L\theta_0 = 0;\ r = 0,\ d\theta_0/dr = 0;\ r = 1,\ d\theta_0/dr = 0 \\ &L\theta_1 = F(\theta_0);\ r = 0,\ d\theta_1/dr = 0;\ r = 1,\ d\theta_1/dr + \nu(\theta_0 - \theta') = 0 \\ &L\theta_2 = F^*(\theta_0)\,\theta_1;\ r = 0,\ d\theta_2/dr = 0;\ r = 1,\ d\theta_2/dr + \nu\theta_1 = 0 \\ &L = \frac{1}{r}\frac{d}{dr}\left(r\frac{d}{dr}\right),\quad \nu = \frac{\mathrm{Bi}}{\mathrm{Pe}},\quad F^*(\theta_0) = 1 - \frac{\beta g}{\theta_0^2}\times\exp\left(-g\exp\left(-\frac{\beta}{\theta_0}\right)\right)\exp\left(-\frac{\beta}{\theta_0}\right) \end{aligned} \tag{4.2}$$

The system of Eqs.(4.2) has the property that constants of the preceding approximation are determined in the process of determining the following approximation.

The solution has the form

$$\begin{aligned} &\theta_0 = \theta' - F(\theta_0)/2\nu \\ &\theta_1 = F(\theta_0)(a_1 r^2 - a_2) \\ &\theta_2 = F^*(\theta_0)F(\theta_0)(a_3 r^4 - a_4 r^2 - a_5),\ \ldots \\ &a_1 = \frac{1}{4},\quad a_2 = \frac{F^* + 4\nu}{8(F^* + 2\nu)},\quad a_3 = \frac{1}{64} \\ &a_4 = \frac{a_2}{2},\quad a_5 = a_2^2 + \frac{F^* + 6\nu}{192(F^* + 2\nu)} \end{aligned} \tag{4.3}$$

Values of θ_0 are determined by the algebraic equation (4.3) that represent the equality of heat release and heat transfer in the model of complete intermixing and coincide with the stationary values of temperature obtained in /1/. Coefficients of expansion a_2, a_4, a_5 gave a singularity when

$$F^*(\theta_0) + 2\nu = 0 \tag{4.4}$$

The last equation implies the equality of slope of curves of heat release and heat removal in a model of complete intermixing with respect to temperature. Consequently, the obtained expansion is valid throughout the parameter domain, except the neighborhood of curve defined by the system of equations (4.3) and (4.4). That curve is at the same time the boundary separating the domain of parameters of the total intermixing model with various numbers of stationary modes, i.e. represents a branching line.

Solution of the system of equations form the first of Eqs.(4.3) and (4.4) can be represented in parametric form by the introduction of parameter

$$y = 1 - \theta(1 + 2\nu) + \theta'' + 2\nu\theta'$$

We have

$$\begin{aligned} &\beta^* = -y\ln y\,[\ln g - \ln(-\ln y)]^2 \\ &\theta^* = -y\ln y\,[\ln g - \ln(-\ln y)] + y - 1 \\ &(\beta^* = (1 + 2\nu)\beta,\ \theta^* = \theta'' + 2\nu\theta',\ y \in (0,1)) \end{aligned} \tag{4.5}$$

Similar curves can be constructed also for reactions of any order n, when $\theta^* = \theta^*(\beta^*, g, n)$.

From the parametric representation (4.5) of branching lines follows that the number of stationary modes of the reactor model of total intermixing with respect to temperature depends on the three parameters β^*, θ^* and g. A set of curves (4.5) is shown in Fig.1 for several values of g. Three stationary modes exist for parameters β^* and θ^* from the region bounded by the curve (4.5), two solutions on the curve itself, for other values of parameters the stationary solution is unique. The dash line in Fig.1 corresponds to sufficient estimates of uniqueness of solution (3.10) for β^* and (3.13) for θ^*. The arrows denote the direction of parameter y increase along the branching curve.

Analysis of the asymptotic expansion (4.3) shows that the constructed regions of uniqueness are applicable also for the determination of the number of stationary modes when $\mathrm{Pe} \neq 0$, $\mathrm{Pe} \ll 1$, when parameters θ^* and β^* are at some distance from the branching curve. Consequently, for a reactor model of total longitudinal intermixing there are no new boundaries of nonuniqueness of solution, and only the branching line is deformed, if only $\mathrm{Pe} \ll 1$. The degree of such deformation is insignificant, since in the first approximation, the equation of the branching line is independent of Pe.

In Fig.2 are shown the critical parameters of ignition and extinction (the branching lines of solution) when $\mathrm{Pe} = 0.1$ and $\ln g = 25$ that were obtained as the result of numerical computations using the finite difference approximation of Eqs.(1.2) and (1.4) and the method of ranging. Lines 1, 2 and 3 correspond to values of $\mathrm{Bi} = 0; 0.02; 0.04$.

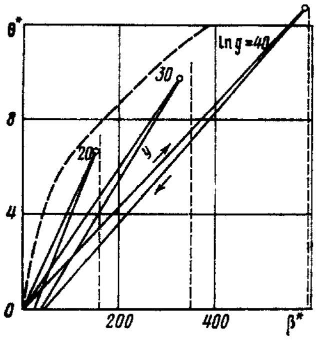

Fig.1

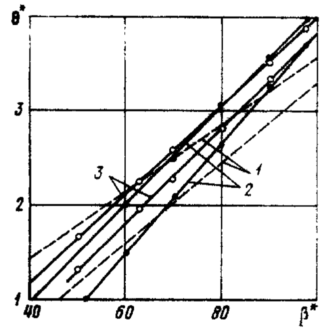

Fig.2

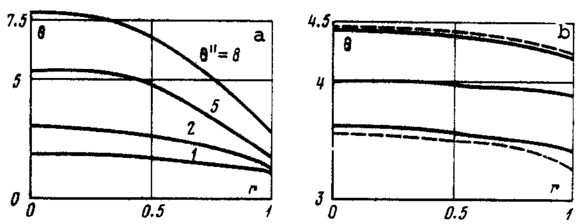

Fig.3

5. Approximate solution with moderate Péclet numbers. Solving the problem (1.2) (1.4) for finite values of the Péclet number by analytical means proved abortive.

The result of numerical computations are given in Fig.3 for parameters $\theta' = 1$; $g = \exp 25$. For parameters $\beta = 25$; $\mathrm{Pe} = 10$; $\nu = 1$ and various θ'' (case a) the solution proved to be unique. In case b when $\beta = 100$; $\mathrm{Pe} = 1$; $\nu = 0.1$, there are three solutions. They are well approximated by the analytical estimate (2.1) shown by the dash line.

These data show that stationary temperature distribution in the reactor is well defined by a parabola whose steepness increases with increase of numbers Pe and Bi.

Let us construct the approximate solution of the problem. Let the temperature distribution along the radius be of the form

$$\theta(r) = B - Ar^2 \tag{5.1}$$

Substituting this distribution into Eqs.(1.2) and (1.4) we reduce their solution, using Green's function (3.2), to the integral equation

$$\theta = \theta' + \mathrm{Pe}\left\{-\int_0^1 G(r, t; \mathrm{Bi})[\varphi(\theta) + \theta]\,t\,dt + \frac{\theta'' + 1}{2}\left(\frac{1}{\mathrm{Bi}} + \frac{1}{2} - \frac{r^2}{2}\right)\right\} \tag{5.2}$$

Introducing the mean temperature $\langle\theta\rangle$ over the radius in conformity with the relation

$$\langle\theta\rangle = 2\int^1 \theta(r)\,r\,dr \tag{5.3}$$

an averaging Eq.(5.1) over the radius, we obtain

$$(1 + 2\nu)\langle\theta\rangle + (\theta'' + 2\nu\theta') = 1 - 2\int_0^1 \varphi t\,dt + \mathrm{Bi}\left\{\int_0^1 (\varphi + \langle\theta\rangle)(t^2 - 1)\,t\,dt + \frac{\theta'' + 1}{4}\right\} \tag{5.4}$$

The integrals appearing in the right-hand side of (5.4) are calculated on the assumption that the temperature distribution over the radius are approximated by Eq.(5.1), whose coefficients A and B are determined by the boundary condition (1.4) in $r = 1$ and from Eq.(5.3)

$$A = \frac{2\,\mathrm{Bi}\,(\langle\theta\rangle - \theta')}{\mathrm{Bi} + 4}, \quad B = \frac{2\,(\mathrm{Bi} + 2)\,\langle\theta\rangle - \mathrm{Bi}\,\theta'}{\mathrm{Bi} + 4} \tag{5.5}$$

Note that the boundary condition (1.4) in $r = 0$ is satisfied for the distribution (5.1) and for any coefficients A and B.

Substituting distribution (5.1) with coefficients (5.5) in the right-hand side of formula (5.4), we obtain for the determination of the mean temperature in the reactor the equation

$$\theta^* = \beta^*\theta^{**} - 1 + \int_0^1 \varphi^*(A^*t + B^* - A^*)\,dt + \mathrm{Bi}\left\{\frac{1}{2}\int_0^1 \varphi^*(A^*t + B^* - A)\,t\,dt - \frac{1}{4}\right\} \quad (5.6)$$

where

$$\varphi^*(x) = \exp(-\exp(\ln g - 1/x)),\ \theta^{**} = \langle\theta\rangle/\beta$$
$$\beta^* = \left[1 + 2\nu + \frac{\mathrm{Bi}\,(\mathrm{Bi}+3)}{3\,(\mathrm{Bi}+4)}\right]\beta$$
$$\theta^* = \theta''\left(1 + \frac{\mathrm{Bi}}{4}\right) + \left[2\nu + \frac{\mathrm{Bi}^2}{12\,(\mathrm{Bi}+4)}\right]\theta'$$
$$\theta^{*\prime} = \beta/\theta',\quad A^* = \frac{2\mathrm{Bi}\,(\theta^{**} - \theta^{*\prime})}{\mathrm{Bi}+4},\quad B^* = \frac{2\,(\mathrm{Bi}+2)\theta^{**} - \mathrm{Bi}\,\theta^{*\prime}}{\mathrm{Bi}+4}$$

The variable β^* and θ^* are determined in such a way that for $\mathrm{Bi} = 0$ they coincide with the previously introduced parameters in (4.5).

Since the numerical computations show that different solutions of problem (1.2), (1.4) correspond the unequal mean temperatures, we can assume that the number of stationary modes of operation of the reactor taking into account the radial temperature gradient, is determined by the number of solutions of Eq. (5.6)

For the determination of the curve which separates regions of the parameters domain with different solutions, we differentiate Eq. (5.6) with respect to θ^{**}. After some transformations, we obtain

$$\beta^* = \frac{\mathrm{Bi}}{A^*}\left\{\int_0^1 \varphi^*(A^*t + B^* - A^*)\,dt - \varphi^*(B^*)\right\} + \quad (5.7)$$
$$\frac{4}{(\mathrm{Bi}+4)\,A^*}\{\varphi^*(B^* - A^*) - \varphi^*(B^*)\} + \frac{\mathrm{Bi}}{\theta^{**} - \theta^{*\prime}}\left\{\int_0^1 \varphi^* t\,dt - \frac{1}{2}\int_0^1 \varphi^*\,dt\right\}$$

Equations (5.6) and (5.7) define parametrically the specified curve $\beta^* = \beta^*(\theta^{**}, g)$ and $\theta^* = \theta^*(\theta^{**}, g)$ on which is possible the change of number of modes. Solution of the input problem (1.2), (1.4) depends on six dimensionless quantities: Pe, Bi, θ', θ'', g and β. But the number of solutions according to (5.6) and (5.7) is determined by only five parameters: Bi, $\theta^{*\prime}$, θ^*, g, β^*.

When $\mathrm{Bi} = 0$, the number of solutions depends only on three parameters θ^*, β^* and g, while Eqs. (5.6) and (5.7) assume the form

$$\beta^* = z^2 \exp(\ln g - z)\exp(-\exp(\ln g - z)) \quad (5.8)$$
$$\theta^* = \beta^* z - 1 + \exp(-\exp(\ln g - z))$$

The branching curve of solution (5.8) represents the same curve as (4.5) but with different parametrization, since for $\mathrm{Bi} = 0$ the obtained solutions coincides with the exact one.

The integral appearing in Eqs. (5.6) and (5.7) can be expressed in terms of two functions $F_1(z)$ and $F_2(z)$ which depend on only one parameter g

$$\int_0^1 \varphi^*(A^*t + B^* - A^*)\,dt = \frac{1}{A^*}[F_1(B^*) - F_1(B^* - A^*)]$$
$$\int_0^1 \varphi^*(A^*t + B^* - A^*)\,t\,dt = \frac{1}{A^{*2}}[F_2(B^*) - F_2(B^* - A^*)] +$$
$$\frac{A^* - B^*}{A^{*2}}[F_1(B^*) - F_1(B^* - A^*)];\quad F_1(z) = \int_0^z \varphi^*(x)\,dx,\qquad F_2(z) = \int_0^z \varphi^*(x)\,x\,dx$$

Tabulating functions $F_1(z)$ and $F_2(z)$ for different values of g using numerical integration it is possible to construct on plane β^*, θ^* regions with different numbers of solutions of problem (1.2), (1.4). By their form they are similar to regions represented in Fig.1 for $\mathrm{Pe} = 0$.

The dependence of maximum value of β^* on the branching curve (the abscissa of point of bifurcation in Fig.1) on parameter Bi determined by formulas (5.6) and (5.7) is shown in Fig.4. The dash line shows the critical values of parameter β of model, above which the phenomenon of igniting and extinguishing becomes impossible. Here $\ln g = 25$.

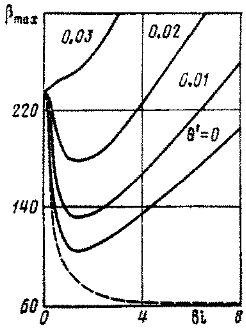

Fig.4

The carried out numerical computations of solution of problem (1.2), (1.4) by the method of ranging and the method of local variation (for large Pe numbers) for various values of parameters show that Eqs.(5.6) and (5.7) adequately define the branching curve of solution for moderate Péclet numbers ($\nu Pe \leqslant 2$) and can be used for the determination of the number of steady modes of reactor operations in the case of ideal displacement with respect to substance and total longitudinal intermixing with respect to energy.

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