STATIONARY OPERATING REGIMES OF CHEMICAL REACTORS

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We investigate the existence and also the number of possible stationary operating regimes of continuous reactors of finite length with a fixed fine-grained catalyzer layer. It is assumed that the effective chemical reaction rate is expressed by a single-valued function of very general form of the temperature and concentration of the primary component in the stream. It is shown in section 1 that in an adiabatic reactor the solution of the direct and inverse problems of finding the stationary regimes always exists and for the inverse problem the solution is unique. In section 2 we establish some sufficient conditions for the uniqueness of the direct problem for the case in which the effective thermal conduction and diffusion coefficients are equal. In section 3 we examine a very simple diffusion model of a reactor with heat removal. An attempt is made to determine the region of variation of the parameters (characterizing the temperature of the supplied mixture, its input rate, heat removal and reactor length) in which the various stationary regimes exist, in particular the low and high temperature regimes and also both of these regimes together.

1. The stationary regimes of the adiabatic reactors in question are usually described [1–3] by the following equations (we have introduced the unknown parameter γ, which characterizes the temperature at the exits from the layer, for purposes of the subsequent investigation):

$$a\frac{d^2u}{d\xi^2}-\frac{du}{d\xi}+f\frac{(u\gamma,\ v\gamma)}{\gamma}=0,\quad b\frac{d^2v}{d\xi^2}-\frac{dv}{d\xi}-f\frac{(u\gamma,\ v\gamma)}{\gamma}=0 \tag{1.1}$$

$$\xi=-l\quad u-a\frac{du}{d\xi}=0,\quad v-b\frac{dv}{d\xi}=\frac{u_m}{\gamma} \tag{1.2}$$

$$\xi=0,\quad u=u_m,\quad \frac{du}{d\xi}=0,\quad \frac{dv}{d\xi}=0 \tag{1.3}$$

$$\left(u=\frac{T-T_-}{T^0\gamma},\quad v=\frac{Ch}{\gamma},\quad \xi=\frac{x-L}{\omega\tau},\quad f(u\gamma,\ v\gamma)=\tau F(T,\ C)h,\quad \gamma=\frac{T_+-T_-}{u_mT^0}\right)$$

$$\left(a=\frac{\varkappa}{w^2\tau},\quad b=\frac{D}{w^2\tau},\quad \frac{1}{\tau}=F(T_-,\ C_-),\quad u_m=C_-h,\quad h=\frac{H}{\rho cT^0},\quad l=\frac{L}{w\tau}\right).$$

Here T is temperature; T^0 is a characteristic temperature (for example, T_-); C is the concentration of the primary component in the reacting mixture; T_- and C_- are the temperature and concentration far ahead of the catalyzer layer; w is the filtration velocity; $F \geq 0$ and H are the effective rate and thermal effect of the chemical reaction; ρc = const is the heat content per unit volume; $\varkappa$ and D are the effective longitudinal thermal conduction and diffusivity; L is the length of the catalyzer layer; T_+ is the temperature at the exit from this layer (an unknown quantity).

From (1.1) and condition (1.2) follows

$$a\frac{du}{d\xi}+b\frac{dv}{d\xi}-u-v+\frac{u_m}{\gamma}=0. \tag{1.4}$$

From (1.4) on the basis of (1.3) we find that $v=u_m(1-\gamma)/\gamma$ for $\xi = 0$. Since $v \geq 0$, then $0\leqslant\gamma\leqslant 1$. If we take u as the independent variable, $p=du/d\xi$, and v and ξ as the sought functions, and if in place of the second equation of (1.1) we take (1.4), then problem (1.1)–(1.3) can be written in the form

$$\frac{dp}{du}=\frac{p\gamma-f(u\gamma,\ v\gamma)}{ap\gamma},\quad \frac{dv}{du}=\frac{(u+v-ap)\gamma-u_m}{bp\gamma},\quad \frac{d\xi}{du}=\frac{1}{p} \tag{1.5}$$

$$u=u_m,\ p=0,\ v=u_m(1-\gamma)/\gamma,\ \xi=0 \tag{1.6}$$

$$u=ap,\ \xi=-l. \tag{1.7}$$

The last condition in (1.2) is satisfied automatically, since it is taken into account in (1.6).

For any smooth, single-valued function $f(u\gamma, v\gamma)$, satisfying

$$f = \partial f / \partial u = 0,\ \partial f / \partial v > 0 \text{ for } v\gamma = 0;\ 0 < f < \infty \text{ for } 0 < v\gamma < \infty \quad (0 \leqslant u\gamma \leqslant u_m) \tag{1.8}$$

(we first assume that H > 0) we show that:

a) the inverse problem (γ given, l to be found) for the system (1.5) – (1.7) always has a unique solution;

b) the direct problem (l given, γ to be found) always has a solution, and for the semi-infinite reactor ($l = \infty$) it is unique.

For given γ problem (1.5), (1.6) is the Cauchy problem. At the point

$$u = u_m,\ p = 0,\ v = v_m = u_m (1 - \gamma) / \gamma,\ \xi = 0$$

there is a singularity (the numerator and denominator in the second equation of (1.5), and for $\gamma = 1$ in the first equation as well, vanish). If $\gamma = 1$ this is a singular point. From this point there emanate three integral curves each for p, v, and ξ, two of which yield $\xi > 0$, which contradicts condition (1.7). There remains one pair of curves with slopes $0 < k_1 < \infty$ and $0 < k_2 < \infty$ (on the basis of (1.8)), yielding near $u = u_m$

$$p = k_1 (u_m - u),\ v = k_2 (u_m - u),\ \xi = -\infty. \tag{1.9}$$

If $0 \leqslant \gamma < 1$, we write the first two equations of (1.5) relative to the derivatives du/dp and dv/dp. The right-hand sides in the resulting equations vanish for $u = u_m,\ v = v_m,\ p = 0$ and have no singularities. If we seek the solution of these equations in the vicinity of u_m in the form of series in p, then after converting to the original variables and by analogy with the preceding analysis discarding the solution with $\xi > 0$, we obtain the following expressions for $p(u, \gamma), v(u, \gamma)$ and $\xi(u, \gamma)$ near $u = u_m$ (to within infinitesimals of higher order):

$$p = \sqrt{2f_m / a\gamma}\,(u_m - u)^{1/2}, \quad v = v_m + a / b\,(u_m - u)$$
$$\xi = -\sqrt{2a\gamma / f_m}\,(u_m - u)^{1/2} \quad (f_m = f(u_m\gamma, v_m\gamma),\ v_m = u_m(1 - \gamma)/\gamma). \tag{1.10}$$

In accordance with (1.9), (1.10) the curves of p and v are positive near $u = u_m$ and retain this sign for $0 \leqslant u < u_m$, since otherwise there would be a point where either $p = 0,\ dp / du \geqslant 0,\ v > 0$, or $v = 0,\ dv / du \geqslant 0,\ p \geqslant 0$, which contradicts (1.5). Since $p > 0,\ 0 < f < \infty$, the curve $p(u,\gamma)$ must of necessity reach the straight line $p = u/a$ (in accordance with (1.5) it cannot turn or have a vertical asymptote) and cross this line only once, since $-\infty < dp / du < 1/a$ in accordance with (1.5).

Thus for any given $0 \leqslant \gamma \leqslant 1$ the solution of the problem (1.5), (1.6) exists and yields the unique values

$$u_0(\gamma) = ap(u_0, \gamma) \geqslant 0, \quad l(\gamma) = -\xi[u_0(\gamma), \gamma] = \int_{u_0}^{u_m} \frac{du}{p} \geqslant 0, \tag{1.11}$$

i.e., the inverse problem (1.5)–(1.7) has a unique solution (u_0 will be the value of u at the entrance to the layer).

We note that in the design of reactors the solution of the inverse problem is meaningful, since it yields the value of the reactor length for which there exist regimes with given maximum temperature or the required quantity of the resulting product.

According to (1.9), for $\gamma = 1$ $l = \infty$. According to (1.10), as $\gamma \to 0$, $p \to \infty$ near u_m; hence $u_0 \to u_m,\ l = -\xi(u_0) \to 0$. The solution of problem (1.5), (1.6) depends continuously on the parameter γ. Therefore, with variation of γ from 0 to 1 the quantity l fills the interval $[0, \infty]$ continuously, i.e., for any $l \geq 0$ there is always at least one value of $0 \leqslant \gamma \leqslant 1$, for which problem (1.5)–(1.7) has a solution. For $l = \infty$ this value ($\gamma = 1$) will be unique, since if $\gamma \neq 1$, then according to (1.10), (1.11). $l < \infty$

Thus, in the adiabatic reactor of arbitrary length l there is always at least one, and for $l = \infty$ only one stationary regime.

In the case H < 0 this analysis remains completely valid except that

$$-\infty < j \leqslant 0,\ u_m < 0,\ u_m \leqslant u \leqslant 0,\ v \leqslant 0,\ p \leqslant 0 \quad (H < 0).$$

2. As is known [4,5], the direct problem may not be unique. Let us establish for a = b the sufficient conditions for its uniqueness. (Other sufficient conditions, effective for small a or l, were obtained in [6] with the aid of the eigenvalue problem.)

Integrating (1.4) relative to u + v with the use of condition (1.3), we obtain $v = u_m / \gamma - u$. Then the system (1.5)–(1.7) takes the form

$$\frac{dp}{du} = \frac{p\gamma - \varphi(u\gamma)}{ap\gamma}, \quad \frac{d\xi}{du} = \frac{1}{p} \tag{2.1}$$

$$u = u_m,\ p = 0,\ \xi = 0; \quad u = ap,\ \xi = -l. \tag{2.2}$$

Differentiating (1.11) and (2.1) with respect to γ; we obtain

$$l_\gamma = \frac{dl}{d\gamma} = -\left(\frac{\partial \xi}{\partial \gamma}\right)_{u=u_0} - \left(\frac{d\xi}{du}\right)_{u=u_0} \frac{du_0}{d\gamma} = -\xi_\gamma(u_0) - \frac{ap_\gamma(u_0)\gamma}{\varphi(u_0\gamma)} \tag{2.3}$$

$$\frac{dp_\gamma}{du} = -\frac{\chi(u\gamma)}{ap\gamma^2} + \frac{\varphi(u\gamma)}{ap^2\gamma} p_\gamma, \quad \frac{d\xi_\gamma}{du} = -\frac{p_\gamma}{p^2} \quad \left(p_\gamma = \frac{\partial p}{\partial \gamma}\right) \tag{2.4}$$

$$\chi(\vartheta) = \vartheta\varphi'(\vartheta) - \varphi(\vartheta) \quad (0 \leqslant \vartheta \leqslant u_m\gamma,\ \vartheta = u\gamma). \tag{2.5}$$

According to (1.10), in the vicinity of u = u_m for $0 \leqslant \gamma < 1$

$$p_\gamma = \left(\frac{u_m - u}{2a\varphi_m\gamma^3}\right)^{1/2} \chi(u_m\gamma), \quad \xi_\gamma = \left(\frac{a(u_m - a)}{2\varphi_m{}^3\gamma}\right)^{1/2} \chi(u_m\gamma)\,(\varphi_m = \varphi\ (u_m\gamma)). \tag{2.6}$$

If $\chi(\vartheta) \leqslant 0$ for $0 \leqslant \vartheta \leqslant u_m\gamma$, then in accordance with (2.6) $p_\gamma \leqslant 0$, $\xi_\gamma \leqslant 0$ near u = u_m and if thereafter these inequalities are violated, there would be a point u^0 where $p_\gamma(u^0) > 0$, $dp_\gamma(u^0)/du \leqslant 0$ or $p_\gamma(u^0) \leqslant 0$, $d\xi_\gamma(u^0)/du < 0$, which contradicts (2.4). Consequently, if $\chi(\vartheta) \leqslant 0$ for $0 \leqslant \vartheta \leqslant u_m\gamma$, then $p_\gamma \leqslant 0$, $\xi_\gamma \leqslant 0$ for $0 \leqslant u \leqslant u_m\gamma$, hence in accordance with (2.3) $l_\gamma(\gamma) \geqslant 0$. If $\chi(\vartheta) \leqslant 0$ for $0 \leqslant \vartheta \leqslant u_m$, then $l_\gamma \geqslant 0$ for all $0 \leqslant \gamma \leqslant 1$, i.e., $l(\gamma)$ is a monotonic function and consequently there is a unique solution $0 \leqslant \gamma \leqslant 1$, which provides the given $l \geqslant 0$.

Thus, if $\chi(\vartheta) \leqslant 0$ $(0 \leqslant \vartheta \leqslant u_m)$, i.e.,

$$\sup\,[\varphi'(\vartheta) - \varphi(\vartheta)/\vartheta] \leqslant 0, \quad \vartheta \in [0,\ u_m], \tag{2.7}$$

then the solution of the direct problem (2.1), (2.2) is always unique, i.e., in a reactor of arbitrary length l for any a there exists a unique stationary regime.

For small ϑ the function $\chi(\vartheta) < 0$, therefore the condition (2.7) is equivalent to the absence of (real) odd multiple roots of $\chi(\vartheta)$.

Thus, for example, in the classical case in which

$$\varphi(\vartheta) = h(u_m - \vartheta)\exp[\vartheta / (1 + b_0\vartheta)] \quad (b_0 = RT\_ / E,\ T^0 = RT\_^2 / E), \tag{2.8}$$

the roots of the function $\chi(\vartheta)$ are

$$\vartheta = [u_m - 2b_0 \pm (u_m - 4b_0u_m - 4)^{1/2}][2(b_0{}^2u_m - 1)]^{-1}. \tag{2.9}$$

It follows from (2.9) that if $u_m \leqslant 4/(1 - 4b_0)$, then $\chi(\vartheta)$ has no roots of odd multiplicity, i.e., the solution of the direct problem will be unique in this case.

The equation $\chi(\vartheta) = 0$ is equivalent relative to ϑ to the system $\varphi(\vartheta) = A\vartheta$, $d\varphi / d\vartheta = A$ which defines the tangents to the curve $\varphi(\vartheta)$, passing through the coordinate origin, where the tangent at the inflection point corresponds to the roots of even multiplicity. Therefore, for uniqueness of the stationary regimes it is sufficient that there be no rays from the coordinate origin which cross the curve $\varphi(\vartheta)$ at more than one point. (Thus we have Fig. 1 for the case (2.8).) This statement can be interpreted as follows: the heat release at each reactor section is determined by the function $\varphi_{-}(\vartheta)$, and the heat removal (into the supplied mixture) can be considered to be roughly proportional to ϑ. Therefore the number of possible stationary states of the reactor will then be no more than the maximum number of points of intersection which the curve $\varphi(\vartheta)$ can have with a ray from the coordinate origin.

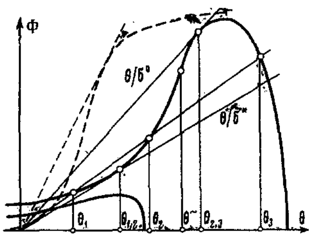

Fig. 1.

In the case $\varphi(\vartheta)\leqslant 0$ the condition that the sign of the function $\chi(\vartheta)$ be constant for $\vartheta\in[u_m, 0]$ is equivalent to condition (2.7), and all the conditions which follow therefrom also will be sufficient for uniqueness of the direct problem (2.1), (2.2). In this case the above analysis is still valid, except that $u_m<0$, $u_m\leqslant u\leqslant 0$, $p\leqslant 0$.

3. Now let us examine the case in which the function $\varphi(u\gamma)$ in (2.1) can change sign. This occurs, for example, for reactors with heat removal. In this case problem (2.1), (2.2) results from seeking the stationary regimes in the case of zero-order reaction (when, for example, no account is taken of the decrease of the active substances along the reactor length, which aids in evaluating the conditions for which combustion will obviously not take place), and also when the C and T fields are similar (which assumes continuous input of the reagents and partial removal of the reaction products through the walls). In this case we use the one-dimensional model, i.e., we assume that either there is ideal transverse mixing or the heat removal is accomplished directly from the reaction zone [1,2], or averaging of the equations with respect to the transverse coordinate is performed [1,7]. A similar problem for the semi-infinite chamber $(l=\infty)$ was examined in [7]. In the present case the problem can be written in the form

$$\frac{dp}{d\theta}=\frac{p-\psi(\theta)}{ap},\quad \frac{d\xi}{d\theta}=\frac{1}{p},\quad \psi(\theta)=\Phi(\theta)-\frac{\theta}{\delta} \tag{3.1}$$

$$\theta=\theta_{+},\ p=0,\ \xi=0;\quad \theta=ap+\theta_{-},\ \xi=-l, \tag{3.2}$$

$$(\theta=(T-T_0)/T^0,\ \Phi(\theta)=\tau F(T)/\rho CT^0,\ 1/\delta=\alpha S\tau/\rho c$$

$$\theta_{+}=(T_{+}-T_0)/T^0,\ \theta_{-}=(T_{-}-T_0)/T^0,\ T^0=RT_0^2/E,\ 1/\tau=F(T_0)/\rho cT^0).$$

Here T_0 is the temperature at the heat-removing surface, S is the area of this surface per unit layer volume, α is the effective heat removal coefficient, $F(T)\geqslant 0$ is the heat release rate, R is a universal constant, E is the activation energy.

Usually, for example in the case of the Arrhenius dependence of the chemical reactor rate on T, the function $\Phi(\theta)$ has the form shown in Fig. 1 (the form of $\Phi(\theta)$ for a zero-order reaction is shown by the dashed curve to markedly reduced scale). Therefore we assume for simplicity that

$$\Phi''(\theta)>0 \text{ for } \theta<\theta^{\sim},\ \Phi''(\theta)<0 \text{ for } \theta>\theta^{\sim}$$
$$|\Phi'(\theta)|<\infty;\ \lim\theta^{-1}\Phi(\theta)=0 \text{ for } \theta\to\infty$$

(in the case in which T and C are similar we have $\Phi(\theta_m)=0,\ \theta<\theta_m$).

Then for $\delta^\circ<\delta<\delta^*$ the function $\psi(\theta)$ has three roots $0<\theta_1<\theta_2<\theta_3$ (Fig. 1), where the roots θ_1, θ_3 diminish together with δ while θ_2 increases, and vice versa. For $\delta<\delta^\circ$ there will be a single root θ_1, and for $\delta>\delta^*$ there will be the single root θ_3. The critical values δ^0 and δ^* and the corresponding points $\theta_{2,3}$ and $\theta_{1,2}$ of merging of the roots θ_2, θ_3 and θ_1, θ_2 are found from the equations

$$\psi(\theta,\ \delta)=0,\quad d\psi/d\theta=0. \tag{3.3}$$

If (3.3) has no positive roots, then $\psi(\theta)$ will have only one root for any δ.

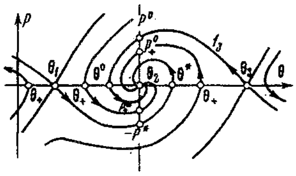

Fig. 2.

Let us assume that in the θp-plane the curves run in the direction of decreasing ξ ($d\xi = d\theta/p < 0$). Then every curve leaving the point $\theta = \theta_+$, $p = 0$ (we denote it by simply θ_+) and crossing the straight line $\theta = \theta_- + \alpha p$ for some $\theta = \theta_0$ obviously ensures a solution of the inverse (θ_+ given, l unknown) problem (3.1), (3.2) and vice versa (θ_0 will be the value of θ at the entrance to the layer).

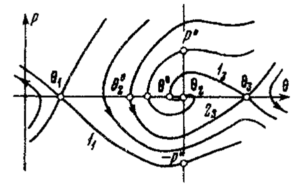

Fig. 3.

In the upper half-plane the motion along the curves takes place from right to left ($p > 0$, hence $d\theta < 0$) and vice versa in the lower half-plane. The points $\theta_1, \theta_2, \theta_3$ ($p = 0$) are singular. Study of the behavior of the curves in the vicinity of these points [7] shows that θ_1 and θ_2 are saddles, while θ_2 is either a node (for $4a\psi'(\theta_2) \leqslant 1$), or a focus (for $4a\psi'(\theta_2) > 1$). In this case the curves approach the point θ_2 and, consequently, there are no solutions with $\theta_+ = \theta_2$ (except for the trivial solution $\theta \equiv \theta_2$ for $\theta_- = \theta_2$). Two branches leave from both points θ_1 and θ_3, while a single branch of the curve leaves from the points $\theta_+ \neq \theta_n$ ($n = 1, 2, 3$) yielding in the vicinity of these points

$$p = \operatorname{sign}\psi_+ \sqrt{\psi_+/a}\,|\theta_+ - \theta|^{1/2}, \quad \xi = -\sqrt{2a/\psi_+}\,|\theta_+ - \theta|^{1/2}, \quad \psi_+ = \psi(\theta_+), \quad \theta_+ \neq \theta_n$$
$$p = k(\theta_+ - \theta), \quad \xi = -\infty \quad (0 < k < \infty), \quad \theta_+ = \theta_1, \theta_3 \;. \tag{3.4}$$

Let $\delta^0 < \delta < \delta^*$, i.e., $\psi(\theta)$ has three roots. Then, as shown in [7], the curves l_1 and l_3 (Figs. 2–4) leaving from θ_1 and θ_3 cross the θ-axis at the points θ^* and θ^0, respectively. Three cases of location of these points, which define the form of the integral curve field, are possible:

1. $\theta_2 \leqslant \theta^* \leqslant \theta_3$, $\theta_1 \leqslant \theta^0 \leqslant \theta_2$ (Fig. 2).
2. $\theta^* = \infty$, $\theta^0 > \theta_1$ (Fig. 3).
3. $\theta^* < \theta_3$, $\theta^0 = -\infty$ (Fig. 4).

Approximate estimates were obtained in [7] for the values of θ^* and θ^0, from which it follows that case 1 occurs for any a if $Q = 0$ (which is equivalent to $\delta = \delta_0$), while case 2 will occur for $a < a^*(\delta)$, if $Q \neq 0$ (a^* decreases with increase of Q). If $a > a^*$, for $Q < 0$ ($\delta < \delta_0$) case 2 will occur, while case 3 will occur for $Q > 0$ ($\delta > \delta_0$). Here

$$Q = \int_{\theta_1}^{\theta_3} \psi(\theta)\,d\theta, \quad \delta_0 = \frac{1}{2}(\theta_3^2 - \theta_1^2)\left[\int_{\theta_1}^{\theta_3} \Phi(\theta)\,d\theta\right]^{-1} . \tag{3.5}$$

The curve leaving the point $\theta_+ < \theta_1$, like the left branch of the curve leaving θ_1 [7], always runs to the left in the upper half-plane. Therefore if $\theta_- \leqslant \theta_+$, it always crosses the straight line $\theta = \theta_- + ap$ for some $\theta = \theta_0 < \theta_+$ (and one time only, since $-\infty < dp/d\theta < 1/a$, for $\theta \leqslant \theta_1$, $p > 0$, in accordance with (3.1)). The value of $\xi(\theta)$ decreases monotonically along the curve, beginning from $\xi = 0$ for $\theta = \theta_+$. Therefore:

1) there is always a unique value of the reactor length $l = -\xi(\theta_0, \theta_+) \geqslant 0$, for which there will exist a regime with any given $\theta_+ \leqslant \theta_1$ and $\theta_- \leqslant \theta_+$, i.e., the inverse problem (3.1), (3.2) has in the region $\theta_+ \leqslant \theta_1$ a unique solution for $\theta_- \leqslant \theta_+$;

2) for any given $l \leqslant l_+^0$ there is always a unique $\theta_- \leqslant \theta_+$, for which there exists a regime with any given $\theta_+ \leqslant \theta_1$ (l_+^0 — is the length corresponding here to the given θ_+ and $\theta_- = -E / RT_0$). We shall see later that with increase of θ_+ the value of l_+^0 increases, approaching infinity as θ_+ approaches θ_1.

In accordance with (3.4) $l = \infty$ for $\theta_+ = \theta_1$ and $l = 0$ for $\theta_+ = \theta_-$. Since the problem solution will obviously depend continuously on θ_+, the values of $l(\theta_+, \theta_-)$ corresponding to the given $\theta_- \leqslant \theta_1$ for different $\theta_+ \in [\theta_-, \theta_1]$ fill continuously the interval $[0, \infty]$. Consequently, for any given $l \geq 0$ and $\theta_- \leqslant \theta_1$ there always exists a regime with $\theta_+ \in [\theta_-, \theta_1]$.
Let us show that there will be only one such regime. To do this we make the following change of variables in (3.1), (3.2):

$$u = (\theta - \theta_-) / \gamma, \quad p = p / \gamma, \quad \gamma = (\theta_+ - \theta_-) / (\theta_1 - \theta_-) \quad (0 \leqslant \gamma \leqslant 1, \ \theta_- \leqslant \theta \leqslant \theta_1). \tag{3.6}$$

Then problem (3.1), (3.2) reduces to the form (2.1), (2.2) and

$$\begin{gathered} \varphi(u\gamma) = \psi(u\gamma + \theta_-) > 0, \quad u_m = \theta_1 - \theta_- \quad (0 < u < u_m), \\ \chi(\vartheta) = \vartheta\psi'(\vartheta + \theta_-) + \psi(\vartheta + \theta_-) = \chi_0(\theta) = (\theta - \theta_-)\psi'(\theta) - \psi(\theta) \quad (\vartheta = u\gamma). \end{gathered} \tag{3.7}$$

Hence $\chi_0(\theta_-) \leqslant 0$, $\chi_0(\theta_1) \leqslant 0$ and $\chi_0'(\theta) = (\theta - \theta_-)\Phi''(\theta) \geqslant 0$ for $\theta_- \leqslant \theta \leqslant \theta_1$, since $\theta_1 < \theta^\sim$.

Consequently, $\chi_0(\theta) \leqslant 0$ on the entire segment $\theta_- \leqslant \theta \leqslant \theta_1$, i.e., $\chi(\vartheta) \leqslant 0$ $(0 \leqslant \vartheta \leqslant u_m)$, and in accordance with section 2 the solution of the direct problem in the region $\theta_+ \leqslant \theta_1$ for $\theta_- \leqslant \theta_1$ is unique.

We find similarly that both the inverse and the direct problems (3.1), (3.2) have in the region $\theta_+ \in [\theta_3, \theta_-]$ a unique solution for $\theta_- \geqslant \theta_3$.

The curve $p(\theta, \theta_+)$, leaving the point $\theta_+ \in (\theta_1, \theta_2)$ like the right branch of the curve leaving θ_1 [7], runs to the right in the lower half-plane, crosses the straight line $\theta = \theta_2$ at the point $p = -p_+^*$, and since $dp / d\theta > 1 / a$ for $\theta_2 < \theta < \theta_3$, $p < 0$, in cases 1 and 3 (Figs. 2, 4) it provides a solution only for $\theta_- \in [\theta_+, \theta_2 + ap_+^*]$. In this case, as follows from Figs. 2 and 4, if $p_+^* \neq 0$, then for $\theta_- > \theta_2 - ap_+^{**}$ intersection with the straight line $\theta = \theta_- + ap$ occurs several times (p_+^{**} is the second crossing of the straight line $\theta = \theta_2$). In other words, for $\theta_+ \in [\theta_1, \theta_2]$, $\theta_- \in [\theta_1, \theta_2 + ap_+^*]$ the inverse problem always exists, and for $\theta_- \in [\theta_2 - ap_+^{**}, \theta_2 + ap_+^*]$ its uniqueness is violated as a result of solutions which pass one or more times through the value $\theta = \theta_2$. The quantities θ (for θ_- sufficiently close to θ_2) or p in these solutions lose their monotonicity, and therefore we call such solutions oscillating. It can be shown from qualitative considerations that these solutions will obviously be unstable. We arbitrarily call the solutions which do not pass through θ_2 monotonic.

Case 2 (Fig. 3) differs in this region in that for $\theta_+ \in [\theta_1, \theta_2^0]$ and for $\theta_- > \theta_2 + ap_+^*$ there is a single oscillating solution which passes through $\theta = \theta_2$ and $\theta = \theta_3$.

Just as before, in the region in question for any given $l \leqslant l_+^0$ there is always a unique value θ_- for which there exists a unique monotonic regime with any given value $\theta_+ \in [\theta_1, \theta_2]$ (l_+^0 corresponds here to the given θ_+ and $\theta_- = \theta_2 + ap_+^*$, i.e., $l_+^0 = -\xi(\theta_2, \theta_+)$).

Similarly to the preceding, we find that monotonic solutions of the direct problem in the region $\theta_+ \in [\theta_1, \theta_2]$ exist for $\theta_- \in [\theta_1, \theta_2]$ for any l and for $\theta_- \in [\theta_2, \theta_2 + ap^*]$ only for $l > l_0$ (l_0 is the smallest value of $l(\theta_+, \theta_-)$ for curves with θ_+ from the interval in question which cross the straight line $\theta = \theta_- + ap$, i.e., in the present case, for which $p_+^* > (\theta_2 - \theta_-) / a$).

Making the replacement (3.6) in (3.1), (3.2), we obtain problem (2.1), (2.2).

For $\theta_- \in [\theta_1, \theta_2]$ we have

$$\begin{gathered} \chi_0(\theta_1) \geqslant 0, \ \chi_0(\theta_-) \geqslant 0; \ \chi_0' \leqslant 0 \ \text{for} \ \theta_1 < \theta < \theta_-, \ \text{it} \ \theta_- \leqslant \theta^\sim; \\ \chi_0' \leqslant 0 \ \text{for} \ \theta_1 < \theta < \theta^\sim, \ \chi_0' \geqslant 0 \ \text{for} \ \theta^\sim < \theta < \theta_2, \ \text{it} \ \theta_- > \theta^\sim. \end{gathered}$$

Therefore if $\theta_- \leqslant \theta^\sim$ or $\theta_- > \theta^\sim$, but $\chi_0(\theta^\sim) \geqslant 0$, i.e., in accordance with (3.7) $\theta_- \leqslant \theta_-^0$ $(\theta_-^0 > \theta^\sim)$, where

$$\theta^0_- = \theta^\sim - \psi(\theta^\sim)/\psi'(\theta^\sim), \tag{3.8}$$

then $\chi_0(\theta) \geqslant 0$ $(\theta_1 \leqslant \theta \leqslant \theta_-)$. However, if $\theta_- > \theta_-^0$, then $\chi_0(\theta)$ has two roots.

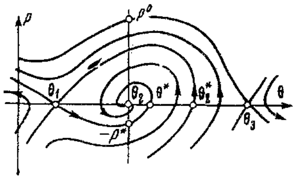

Fig. 4.

For $\theta_- \in [\theta_2, \theta_2 + ap^*]$ the function $\chi_0(\theta)$ (3.7) varies in the interval $[\theta_1, \theta_2]$, since here $\theta_0 \leqslant \theta_2$ always. In this case $\chi_0(\theta_1) > 0$, $\chi_0(\theta_2) \leqslant 0$, i.e., $\chi(\theta)$ for $\theta_1 \leqslant \theta \leqslant \theta_2$ has a single root.

Consequently, in accordance with section 2, if $\theta^\sim \geqslant \theta_2$ or $\theta_-^0 \geqslant \theta_2$, then for $\theta_- \in [\theta_1, \theta_2]$, and in the opposite case for $\theta_- \in [\theta_1, \theta_-^0]$ the direct problem has in the region $\theta_+ \in [\theta_1, \theta_2]$ a unique monotonic solution.

For $\theta_- \in [\theta_-^0, \theta_2]$, if $\theta^\sim < \theta_-^0 < \theta_2$, and also for $\theta_- \in [\theta_2, \theta_2 + ap]$, $l > l_-^0$ it has one or more such solutions, and from the qualitative considerations of section 2 it follows that in the first case there will be no more than three solutions and in the second case no more than two.

Similar results are obtained for the region $\theta_+ \in [\theta_2, \theta_3]$.

Because of lack of space we do not present here the approximate estimates for p^* and p_+^*, nor for the corresponding values of p^0 and p_+^0 in the region $\theta_+ \in [\theta_2, \theta_3]$ (Figs. 2–4), which are obtained similarly to the estimates for θ^0 and θ^* [7]. We simply note that these values increase with increase of a, the size of the corresponding interval, and the value of $|\psi(\theta)|$ on this interval.

If the function $\psi(\theta)$ can be represented on the intervals in question in the form of power-law series, then the values of p^* and p^0 are obtained in the form of series in integral powers of $(\theta_2 - \theta_1)$ and $(\theta_3 - \theta_2)$ respectively (by suitable choice of T^0 we can ensure that the latter are smaller than unity) and p_+^* and p_+^0 in the form of series in powers of $|\theta_2 - \theta_+|^{1/2}$.

Thus, for $\delta^0 < \delta < \delta^*$ we finally have the following:

For $\theta_- < (\theta_1, \theta_2 - ap^0)$, i.e., for $\theta_- < \theta_1$, if $\theta_1 < \theta_2 - ap^0$ and for $\theta_- < \theta_2 - ap^0$, if $\theta_2 - ap^0 < \theta_1$, and also for $\theta_- > (\theta_3, \theta_2 + ap^*)$ in the reactor of arbitrary length l there always exists a unique monotonic regime, and $\theta_+ \in [\theta_-, \theta_1]$ and $\theta_+ \in [\theta_3, \theta_-]$, respectively.

For $\theta_- \in [\theta_1, \theta_2 - ap^0]$ if $\theta_1 < \theta_2 - ap^0$, and also for $\theta_- \in [\theta_2 - ap^0, \theta_2]$, if $l < l^0_-$ monotonic regimes exist only with $\theta_+ \in [\theta_1, \theta_-]$. Similarly, for $\theta_- \in [\theta_2 + ap^*, \theta_3]$, and for $\theta_3 > \theta_2 + ap^*$ and for $\theta_- \in [\theta_2, \theta_2 + ap^*]$, if $l < l^0_-$, there exist regimes only with $\theta_+ \in [\theta_-, \theta_3]$. In this case, if θ^0_- falls in the interval between $\theta^\sim$ and θ_2 then for $\theta_- \in [\theta^0_-, \theta_2]$ the possibility of the existence of several (no more than three) such regimes is not excluded. In the remaining cases these regimes are unique.

In the case $a > a^*(\delta)$ in reactors of sufficient length for $\theta_- < \theta_2 - ap^0$, if $\delta_0 < \delta < \delta^*$ (Fig. 4), and for $\theta_- > \theta_2 + ap^*$, if $\delta^0 < \delta < \delta_0$ (Fig. 3), there are also oscillatory regimes with $\theta_+ \in [\theta^*_2, \theta_3]$ and $\theta_+ \in [\theta_1, \theta^0_2]$ respectively (δ_0 from (3.5)). In the remaining cases mentioned above there exist only monotonic regimes.

For $\theta_- \in [\theta_2 - ap^0, \theta_2 + ap^*]$ and $l \geqslant l^0_-$ (l^0_- decreases as θ_- approaches θ_2 so that $l^0_- = 0$ for $\theta_- = \theta_2$) it is possible to have simultaneously monotonic regimes with $\theta_+ < (\theta_2, \theta_-)$ and with $\theta_+ > [\theta_2, \theta_-]$, while for $\theta_- = \theta_2$ the unstable trivial regime $\theta \equiv \theta_2$ is also possible. Moreover, for $\theta_- \in [\theta_2 - ap^0, \theta_2]$ there will be one or more regimes with $\theta_+ > \theta_2$, and for $\theta_- \in [\theta_2, \theta_2 + ap^*]$ with $\theta_+ < \theta_2$ (from qualitative considerations no more than two). However the regime with $\theta_+ < \theta_-$ for $\theta_- \in [\theta_2 - ap^0, \theta_2]$ and with $\theta_+ > \theta_-$ for $\theta_- \in [\theta_2, \theta_2 + ap^*]$ is unique except for the case in which θ^0_- falls in the interval between $\theta^{\sim}$ and θ_2 and θ_- falls between θ^0_- and θ_2, for which we can expect several (from qualitative considerations no more than three) such regimes.

Here the value $\theta_- = \theta_2 + ap^*$ can be called the ignition temperature, since this is the maximum temperature of the supplied mixture for which the regime with $\theta_+ < \theta_2$ can still exist. With increase of θ only the regime with $\theta_+ > \theta_- > \theta_2 + ap^*$ becomes possible. Similarly, $\theta_- = \theta_2 - ap^0$ can be termed the extinction temperature.

Along with the monotonic solutions in the θ interval in question, for sufficiently large l there may also be oscillating solutions with $\theta_+ \in [\theta_1, \theta_3]$, which pass one or more times through the value θ_2. Their possibility increases with approach of θ_- to θ_2 and increase of a. It follows from qualitative considerations that these solutions will be unstable and lead to one of the monotonic regimes [7].

Now assume that $\delta < \delta^0$, and $\delta > \delta^*$, i.e., that system (3.3) has no solutions. Then $\psi(\theta)$ has only a single positive root θ_1 (or θ_3) and we find similarly to the preceding that in reactors of arbitrary length l for any a and θ_- there exist stationary regimes only with θ_+ located in the interval between θ_- and θ_1 (θ_- and θ_3). For $\delta^{\sim} < \delta < \delta^0$, $\theta_- > \theta^0_-$ ($\delta^{\sim} = 1/\Phi'(\theta^{\sim}) < \delta^0$, and $\theta^0_- > \theta^{\sim}$ from (3.8)), for $\delta > \delta^*$, $\theta_- < \theta^0_-$ (where $\theta^0_- < \theta^{\sim}$) and when (3.3) has no roots, for $\delta > \delta^{\sim}$, $\theta_- < \theta^0_-$ (where $\theta_-^0 < (0, \theta^{\sim})$) one or more of the indicated regimes is possible (from qualitative considerations no more than three). In the remaining cases the regimes are unique.

Thus, the low-temperature regime which is most often used in chemical processing, when the maximum temperature θ_+ reached at the exit from the layer does not exceed θ_1, exists in reactors of arbitrary length for $\delta \leqslant \delta^*$, $\theta_- \leqslant \theta_1$, and $\theta_+ \in [\theta_-, \theta_1]$. If $\delta^0 < \delta < \delta^*$ and $\theta_2 - ap^0 < \theta_1$, then for $\theta_- \in [\theta_2 - ap^0, \ \theta_1]$ in reactors of length $l \geqslant l_-^0$ along with the single low-temperature regime there also exist high-temperature (from qualitative considerations no more than three) regimes with $\theta_+ \in [\theta_2, \theta_3]$. In the remaining cases the low temperature regime is unique if we do not consider the oscillating solutions with $\theta_+ \in [\theta^*_2, \theta_3]$, which are possible in reactors of sufficiently great length for $a > a^*(\delta)$, $\delta_0 < \delta < \delta^*$, where $\delta_0 > \delta^0$ from (3.5). If system (3.3) has no roots, then for any δ for $\theta_- \leqslant \theta_1$ there exists only the regime with $\theta_+ \leqslant \theta_1$. With increase of δ the value of θ_1 increases monotonically.

With reduction of a, and also for sufficiently small l or δ, the region of ambiguity of the solutions becomes smaller. Thus, extending the results obtained in [6] to our problem, we can state that if

$$\Phi'(\theta^{\sim}) < 1/\delta + 1/4 \cdot 1/a \quad \text{or} \quad \Phi'(\theta^{\sim}) < 1/\delta + 1/l,$$

then for any initial temperature θ_- of the supplied mixture there exists in the reactor a unique stationary regime.

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