

CONDITIONS FOR DIFFERENT STEADY STATES
IN AN ADIABATIC CONTINUOUS-FLOW REACTOR
WITH A CATALYST LAYER

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An adiabatic reactor with continuous flow and with a stationary fine-grained catalyst layer is examined. The mixture which passes through this layer undergoes chemical reaction on the surface of the grains. The reaction there is accompanied by liberation of heat and change in the concentration of the mixture with subsequent heat and mass exchange between this surface and the flow. The rate of the reaction depends on the temperature and concentration of the reagents, in which the relationship to the temperature is markedly nonlinear.

Similar systems are widely used in chemical technology and also in heterogeneous combustion. A special feature of these systems is the nonuniqueness of the steady states. This nonuniqueness can depend on a number of causes, especially longitudinal mixing in the flow when the length of the reactor is limited (which is examined in a number of works, for example in [1-5]), heat removal through the walls (which was shown in [5, 6]), and also resistance to heat and mass exchange between the surface of the grains and the flow. The latter leads here to the existence of principally different steady states: in the case of kinetic conditions, for example, the temperature in the flow and in the catalyst are similar, but diffusion conditions, on the other hand, are accompanied by strong heating up (ignition) of the catalyst. Hence the transition from one system to the other usually occurs with a jump.

In practice, kinetic conditions are used in some cases, and in other cases diffusion conditions are used (in some industrial processes the temperature of the catalyst and that of the flow differ by hundreds of degrees, but in the majority of cases, on the other hand, a significant heating of the catalyst is inadmissible).

Qualitative research on the corresponding steady-state equations is carried out below, with a view to determining the regions of variation of the parameters in which there exists each of the conditions mentioned above, especially regions in which both kinetic and diffusion conditions could take place and also regions in which, on the other hand, there is not one stable steady state. Regions are also shown in which what are known as upper diffusion conditions are possible, in which the temperature of the catalyst exceeds the adiabatic heating of the reacting mixture in the case of full conversion.

A similar problem for an individual grain (or cell), with the assumption that the temperature and concentration in the main flow are known, was investigated previously (for example, in [7-10]). In [11-13] numerical integration of the corresponding nonsteady-state equations for the whole reactor was carried out, and the possibility of plurality of steady conditions, caused by the nonuniqueness of steady states in a single grain, was shown.

We will also note that in research and calculation of chemical reactors with continuous flow and with a stationary fine-grained catalyst layer, no distinction is made between the values of the temperature and

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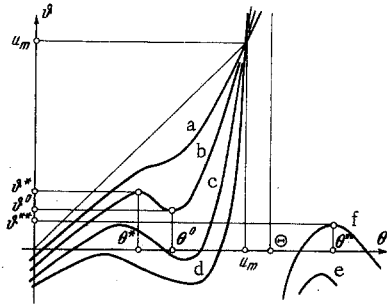


Fig. 1

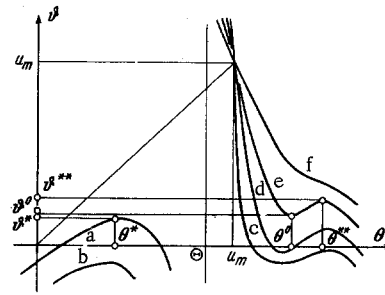


Fig. 2

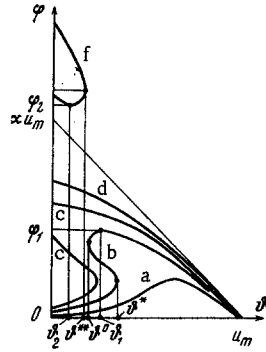


Fig. 3

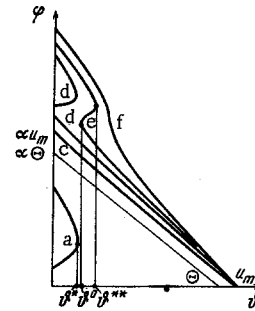


Fig. 4

concentration in the main flow and on the surface of the grains. This reduces the number of equations, but this is permissible only for kinetic conditions. In some works which deal with what are known to be diffusion conditions, it is assumed that full conversion of the substances which are found on the grains takes place. In this case the number of equations is also reduced, and the latter will be linear.

The results given below help in evaluating the limitations of the applicability of both the above-mentioned assumptions, the first of which, in particular, excludes the possibility of "ignition" of the catalyst, and the second excludes the possibility of its "extinction."

The steady-state processes in the reactor examined are described by a system of equations of convective heat transfer and diffusion in the basic flow taking into account the heat and mass transfer from the surface of the grains and the equations of the thermal and material balance of the grain (it is assumed that an exothermal reaction of the first order takes place there). If a number of usual [8-14] simplifying assumptions are adopted, especially the constancy of the physical properties, the quasihomogeneity of both phases, the uniformity of the conditions in the lateral direction, and also the absence of thermal conduction in the layer itself (in [15] it is shown, for example, that in the case of liquid flow and in the case of sufficiently high speeds of the gas flow it is possible to neglect it), then the above-mentioned system can be written in the form

$$\kappa \frac{d^2 T}{dx^2} - w \frac{dT}{dx} + \frac{\alpha_1}{\rho c} (T_1 - T) S = 0, \quad D \frac{d^2 C}{dx^2} - w \frac{dC}{dx} + \beta_1 (C_1 - C) S = 0 \quad (1)$$

$$\alpha_1 (T_1 - T) = HC_1 K(T_1), \quad \beta_1 (C_1 - C) = -C_1 K(T_1) \quad (2)$$

$$x = 0, \quad wT - \kappa dT/dx = wT_-, \quad wC - DdC/dx = wC_- \quad (3)$$

$$x = L, \quad dT/dx = 0, \quad dC/dx = 0 \quad (4)$$

Here, T and C are the temperature of the mixture and the concentration of the determining reagent in the main flow, T_1 and C_1 are the temperature and concentration on the surface of the catalyst grains, x is the three-dimensional coordinate, κ and D are the effective coefficients of the thermal conductivity and diffusion in the flow, w is the speed of filtration, α_1 , β_1 are the coefficients of heat and mass transfer from the surface for unit volume, T_- and C_- are the temperature and concentration at a distance before the catalyst layer, $H > 0$ and $K(T_1)$ are the heat and rate constant of the chemical reaction, which usually has the form of an Arrhenius relationship, that is,

$$K(T_1) = k_0 \exp[-E/RT_1] \quad (5)$$

where E is the energy of activation and R is the universal constant.

We will make the following substitution of variables:

$$u = \frac{\vartheta}{\gamma}, \quad U = \frac{\theta}{\gamma}, \quad v = \frac{s}{\gamma}, \quad \xi = \frac{x-L}{w\tau}, \quad \vartheta = \frac{(T-T_-)E}{RT_-^2}, \quad \theta = \frac{(T_1-T_-)E}{RT_-^2} \quad (6)$$

$$s = Ch, \quad h = \frac{HE}{\rho c RT_-^2}, \quad \frac{1}{\tau} = K(T_-)S, \quad u_m = C_-h, \quad \gamma = \frac{\vartheta_+}{u_m}$$

Here, ϑ and θ are the dimensionless temperature in the flow and on the surface of the grains, u_m is the adiabatic initial heating of the mixture in the case of full conversion, and ϑ_+ is the maximum value of ϑ , reached at the exit from the layer (unknown magnitude). We will note that $0 \leq \vartheta_+ \leq u_m$, so that $0 \leq \gamma \leq 1$.

Equations (1) and (2) have the first integral which, taking (3) and (6) into account, can be written in the form

$$a \frac{du}{d\xi} + b \frac{dv}{d\xi} - u - v + \frac{u_m}{\gamma} = 0 \quad \left(a = \frac{\kappa}{w^2\tau}, \quad b = \frac{D}{w^2\tau} \right) \quad (7)$$

In accordance with (6), (7), and (4) we obtain

$$u = u_m, \quad v = u_m(1-\gamma)/\gamma \quad \text{for } \xi = 0 \quad (8)$$

We will write (1) to (4) in new variables, taking as the unknown functions $p = a u / d\xi$, v , and ξ , and we will take the value u as the independent variable. Here we will substitute the second equation in (1) by the integral (7) and the boundary condition (4) by the condition (8); we will eliminate C_1 from (2). Then the problem considered can be presented in the form

$$\frac{dp}{du} = 1 - \frac{a\psi(u\gamma, v\gamma)}{p\gamma}, \quad \frac{dv}{du} = \frac{(u+v)\gamma - u_m}{\lambda p\gamma} - \frac{1}{\lambda}, \quad \frac{d\xi}{du} = \frac{a}{p} \quad (9)$$

$$\psi(\vartheta, s) = \alpha [\theta(\vartheta, s) - \vartheta], \quad \vartheta = \theta - \sigma k(\theta)/[\beta + k(\theta)] \quad (10)$$

$$u = u_m, \quad p = 0, \quad v = u_m(1-\gamma)/\gamma, \quad \xi = 0; \quad u = p, \quad \xi = -l \quad (11)$$

Here

$$\alpha = \frac{\alpha_1 S \tau}{\rho c}, \quad \beta = \beta_1 S \tau, \quad \sigma = \frac{\beta}{\alpha}, \quad \lambda = \frac{b}{a}, \quad k(\theta) = \exp \frac{\theta}{1 + b_0 \theta} \quad (12)$$

$$b_0 = \frac{RT_-}{E}, \quad l = \frac{L}{w\tau}$$

The second relationship in (10) is an implicit form of the function $\theta(\vartheta, s)$ through which the effective rate of the reaction $\psi(\vartheta, s)$ in (9) is determined in accordance with the first relationship in (10).

In real processes $b_0 \theta$ is usually very small, so that without introducing large errors, $k = e^\theta$ can be adopted. Moreover, if the second equation in (9) is integrated, considering p to be known, it is then possible to obtain the following relationship:

$$v = \frac{u_m}{\gamma} - u + \left(\frac{1}{\lambda} - 1 \right) \int_u^{u_1} \exp \left[- \int_u^{u_1} \frac{du_2}{\lambda p} \right] du_1$$

Hence

$$s = s_1 \quad \text{for } \lambda = 1, \quad s_1 < s < s_2 < s_1/\lambda \quad \text{for } \lambda < 1 \quad (s_1 = u_m - \vartheta)$$

$$s_1/\lambda < s_2 < s < s_1 \quad \text{for } \lambda > 1 \quad (s_2 = u_m [\lambda + (1-\lambda)\gamma] / \lambda - \vartheta / \lambda) \quad (13)$$

Then, when $\lambda = 1$ (which can be adopted quite often), the problem (9) to (11) is reduced to the form

$$\frac{dp}{du} = 1 - \frac{a\varphi(u\gamma)}{p\gamma}, \quad \frac{d\xi}{du} = \frac{a}{p}, \quad \varphi = \alpha [\theta(\vartheta) - \vartheta] \quad (14)$$

$$\vartheta = \theta - \frac{\Phi(\theta)}{\alpha}, \quad \Phi = \frac{\beta(u_m - \theta)}{\beta e^{-\theta} + 1 - \sigma} \quad (15)$$

$$u = u_m, \quad p = 0, \quad \xi = 0; \quad u = p, \quad \xi = -l \quad (16)$$

TABLE 1

	Fig.	Region of variation of the parameters
1	1, ae; 3, a	$u_m < (A, B_1, \Theta)$, i.e., $u_m < A, u_m < B_1$ (for $\beta > e^2$), $u_m < \Theta$
2	1, be; 3, b	$\beta > e^2, \sigma < \sigma_3, A < u_m < B_1$
3	1, ce; 3, c	$\beta > e^2, \sigma < \sigma_3, B_1 < u_m < (B_2, \Theta)$
4	1, bf; 3, bf	$\beta > e^2, \sigma_2 < \sigma < 2, (B_1, A) < u_m < \Theta$
5	1, af; 3, af	$\beta > e^2, \sigma_3 < \sigma < \sigma_6, B_1 < u_m < (A, \Theta)$
6	1, de; 3, d	$\beta > e^2, \sigma < \sigma_1, B_2 < u_m < \Theta$ or $\beta > e^2, \sigma < 2, A < u_m < \Theta$
7	2, af; 4, af	$\beta > e^2, \sigma_1 < \sigma < \sigma_4, (A, \Theta) < u_m < B_2$
8	2, ae; 4, ae	$\beta > e^2, 2 < \sigma < \sigma_3, \Theta < u_m < (A, B_2)$
9	2, bd; 4, d	$\beta > e^2, \sigma > \sigma_5, (\Theta, B_1) < u_m < B_2$
10	2, be; 4, e	$\beta > e^2, \sigma > \sigma_4, B_2 < u_m < A$
11	2, bc; 4, c	$\beta > e^2, \sigma > \sigma_6, \Theta < u_m < B_1$ or $\beta < e^2, \sigma > 2, \Theta < u_m < A$
12	2, bf; 4, f	$u_m > (A, B_2, \Theta)$

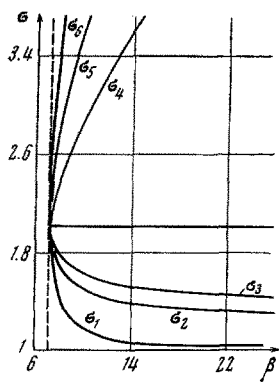


Fig. 5

The denominator in (15), when $\sigma < 1$, does not become zero, but when $\sigma > 1$, it has one root Θ [see (18)]. We find (Figs. 1 and 2) from (15) that

$$\begin{aligned} \vartheta(\Theta \pm 0) &= \mp \infty \text{ for } \Theta > u_m, \quad \vartheta(\Theta \pm 0) = \pm \infty \text{ for } \Theta < u_m, \\ \vartheta(\Theta) &< \Theta \text{ for } \Theta < (u_m, \Theta), \quad \vartheta(\Theta) > u_m \text{ for } \Theta \in (u_m, \Theta), \\ \vartheta(\Theta) &< u_m - (\Theta - u_m) / (\sigma - 1) \text{ for } \Theta > (u_m, \Theta), \quad \vartheta(u_m) = u_m \end{aligned}$$

We note that when $\sigma < 1$ it is possible to assume that $\Theta = \infty$.

The extreme values of the function $\vartheta(\theta)$ correspond to the points of the intersection of the curves

$$\mu_1(\theta) = \beta + \beta^{-1}(1 - \sigma)e^{2\theta}, \quad \mu_2(\theta) = \sigma(u_m - 2\sigma^{-1} + 1 - \theta)e^{\theta} \quad (17)$$

These curves osculate in the case of $u_m = A$ (σ, β) at the point $\theta = T(\beta)$, but if $\delta > 1$, then again in the case of $u_m = \Theta(\sigma, \beta)$ at the point $\theta = \Theta(\sigma, \beta)$. Here

$$A(\sigma, \beta) = \ln \beta + 4\sigma^{-1} - 2, \quad T(\beta) = \ln \beta, \quad \Theta(\sigma, \beta) = \ln \beta - \ln(\sigma - 1) \quad (18)$$

Hence, on the basis of the form of the curves μ_1 and μ_2 , it can be concluded that if $\sigma < 1$, then when $u_m < A$ the latter do not intersect, that is, $\vartheta(\theta)$ does not have extreme values (Fig. 1, curve a, when $\Theta = \infty$). In the case $u_m > A$ there are two intersections: when $\theta = \theta^*$ and when $\theta = \theta^0$, that is, $\vartheta(\theta)$ will have two extreme values: in the case of $\theta = \theta^*$ it is maximum (since $d\vartheta/d\theta > 0$ when $\theta = -\infty$), and for $\theta = \theta^0$ it is minimum (Fig. 1, curves b, c, and d when $\Theta = \infty$).

Similarly, if $1 < \sigma < 2$, then when $u_m < A$ the curve $\vartheta(\theta)$ has one extreme value (maximum) in the case of $\theta = \theta^{**}$. Here the curve consists of two branches: a and e or a and f (Fig. 1, ae, af). In the case $A < u_m < \Theta$, there are three extreme values: the maxima in the cases $\theta = \theta^*$, $\theta = \theta^{**}$, and the minimum when $\theta = \theta^0$ (Fig. 1, be, bf, ce, cf, de, df), and when $u_m > \Theta$ there is one extreme value (maximum) when $\theta = \theta^*$ (Fig. 2, af, bf). Here

$$\theta^* < T(\beta), \quad T(\beta) < \theta^0 < \Theta(\sigma, \beta), \quad \theta^{**} > \Theta(\sigma, \beta) \quad (\sigma < 2) \quad (19)$$

If $\sigma > 2$, then, similarly, when $u_m < \Theta$, we have Fig. 1, ae, af; when $\Theta < u_m < A$, we have Fig. 2, ac, ad, ae, bc, bd, be; and when $u_m > A$, we have Fig. 2, af, bf. Here

$$\theta^* < \Theta(\sigma, \beta), \quad \Theta(\sigma, \beta) < \theta^0 < T(\beta), \quad \theta^{**} > T(\beta) \quad (\sigma > 2) \quad (20)$$

We will investigate the position of the points $\vartheta^0 = \vartheta(\theta^0)$, $\vartheta^* = \vartheta(\theta^*)$, and $\vartheta^{**} = \vartheta(\theta^{**})$ (Figs. 1 to 4). In accordance with (15), with increase of u_m or σ and also with decrease of β (this also means α in the case of constant σ), the left branch of the curve $\vartheta(\theta)$ in Figs. 1 and 2 drops, but the right branch rises. Therefore, in accordance with the preceding,

$$\begin{aligned} \max \vartheta^* &= \max \vartheta^0 = M_1, \quad \min \vartheta^0 = \max \vartheta^{**} = M_2 \text{ for } u_m \leq \Theta \quad (\sigma < 2) \\ \max \vartheta^0 &= \max \vartheta^{**} = M_1, \quad \max \vartheta^* = \min \vartheta^0 = M_2 \text{ for } u_m \geq \Theta \quad (\sigma > 2^*) \\ M_1 &= \ln \beta - 2 = \vartheta(T) \text{ for } u_m = A, \quad M_2 = \Theta - \beta^{-1}e^{\Theta} - 1 = \vartheta(\Theta) \text{ for } u_m = \Theta \end{aligned} \quad (21)$$

Since in the case $u_m > \Theta$, $\sigma < 2$ and in the case $u_m < \Theta$, $\sigma > 2$, the curve $\vartheta(\theta)$ has only one extreme value, which, on the basis of (21), can be written

$$\vartheta^{**} < \vartheta^0 < \vartheta^* \text{ for } u_m < \Theta \text{ (Figs. 1, 3), } \vartheta^* < \vartheta^0 < \vartheta^{**} \text{ for } u_m > \Theta \text{ (Figs. 2, 4)} \quad (22)$$

Hence it follows in particular that $\theta(\vartheta)$ and, consequently, also $\varphi(\vartheta)$ have no more than three values. Moreover, in accordance with (21) and (22)

$$\theta^{\circ} < 0, \theta^* < 0, \theta^{**} < 0 \text{ for } \beta < e^2 \quad (23)$$

If $\beta > e^2$, then the maximum values of the magnitudes $\vartheta^*, \vartheta^{\circ}$ for $\sigma < 2$ and $\vartheta^{\circ}, \vartheta^{**}$ for $\sigma > 2$, obtained when $u_m = A$, are positive. With increase of u_m in the first case and with decrease of u_m in the second case, these magnitudes decrease. The values $u_m = B$ and $\theta = \theta_0$ at which one of the magnitudes $\vartheta^{\circ}, \vartheta^*$, or ϑ^{**} becomes zero, that is, $\vartheta = \vartheta' = 0$, are determined in accordance with (15) from the following relationships:

$$\beta = (\theta_0 - 1)^{-1} e^{\theta_0}, \quad b = (\theta_0 - 1)^{-1} \theta_0^2, \quad B = b\sigma^{-1} \quad (24)$$

From (24) for $\beta > e^2$ we obtain two values $\theta_0^{(1)}(\beta) > 2$ and $\theta_0^{(2)}(\beta) < 2$, and through these we also obtain $4 < b_1(\beta) < b_2(\beta)$ and B_1 and B_2 which correspond to them. We will note that in order to construct graphs $\theta_0^{(1,2)}(\beta)$ and $b_{1,2}(\beta)$ it is sufficient to construct the corresponding curves $\beta(\theta_0)$ and $\beta(b)$ from (24), where

$$\beta(b) = [1/2b(1 \pm \sqrt{1-4b^{-1}}) - 1]^{-1} \exp\{1/2b(1 \pm \sqrt{1-4b^{-1}})\} \quad (25)$$

It is possible also to obtain the following approximated expressions for $B_{1,2}$:

$$B_1 \approx \sigma^{-1} [\ln \beta + 1 + \ln(\ln \beta + 1)], \quad B_2 \approx \sigma^{-1} [\beta e^{-1} + 1 + 1/2(\beta e^{-1} + 1)^{-1}] \quad (26)$$

From (18) and (24) it can be found that

$$\begin{aligned} \theta_0^{(2)} < \theta_0^{(1)} < \theta \text{ for } \sigma < \sigma_2(\beta), \quad \theta < \theta^{(2)} < \theta_0^{(1)} \text{ for } \sigma > \sigma_5(\beta) \\ \theta_0^{(2)} < \theta, \theta_0^{(1)} > \theta \text{ for } \sigma_2 < \sigma < \sigma_5 \end{aligned} \quad (27)$$

Here σ_2 and σ_5 are functions obtained from

$$\beta(\sigma) = (\sigma - 1) \exp[\sigma / (\sigma - 1)]$$

where $\sigma < 2$ and $\sigma > 2$, respectively.

From (27), (19), and (20) it follows that if $\sigma < \sigma_2$, then when $u_m = B_1$, $\theta_0^{(1)} = \theta^{\circ}, \vartheta^{\circ} = 0$, and when $u_m = B_2$, $\theta_0^{(2)} = \theta^*, \vartheta^* = 0$. If $\sigma_2 < \sigma < \sigma_5$, then, in distinction from the case where $u_m = B_1$, $\theta_0^{(1)} = \theta^{**}, \vartheta^{**} = 0$. If $\sigma > \sigma_5$, then when $u_m = B_1$, $\theta_0^{(1)} = \theta^{**}, \vartheta^{**} = 0$, and when $u_m = B_2$, $\theta_0^{(2)} = \theta_0, \vartheta^{\circ} = 0$.

Similarly we will obtain $(\sigma_{1-7}(\beta))$ given in Fig. 5)

$$\begin{aligned} A < B_1 < B_2 < \theta \text{ for } \sigma < \sigma_1, \quad A < B_1 < \theta < B_2 \text{ for } \sigma_1 < \sigma < \sigma_3 \\ B_1 < A < \theta < B_2 \text{ for } \sigma_3 < \sigma < 2, \quad B_1 < \theta < A < B_2 \text{ for } 2 < \sigma < \sigma_4 \\ B_1 < \theta < B_2 < A \text{ for } \sigma_4 < \sigma < \sigma_5, \quad \theta < B_1 < B_2 < A \text{ for } \sigma > \sigma_6 (\beta > e^2) \\ A < \theta \text{ for } \sigma < 2, \quad \theta < A \text{ for } \sigma > 2 (\beta < e^2) \end{aligned} \quad (28)$$

In accordance with (27) and (28), on the basis of the statement given above it is possible to establish twelve different types of curves $\vartheta(\theta)$ and consequently also $\theta(\vartheta)$ (Figs. 1 and 2) and also $\varphi(\vartheta)$ from (14) (Figs. 3 and 4), which include all the possible values of u_m , σ , and β (Table 1). We note that $\varphi(\vartheta)$ as seen from the last relationship of (14) is expressed through $\theta(\vartheta)$ in an elementary manner. In particular, it follows at once from this that $\theta(\vartheta)$ and $\varphi(\vartheta)$ have generally vertical tangents (where $\vartheta = \vartheta^*, \vartheta^{\circ}, \vartheta^{**}$). For simplicity the points u_m , θ , and αu_m in Figs. 1-4 are fixed. Hence it is necessary to mention that in the case of different u_m , θ , and α they have a different value. The maximum φ_1 and the minimum φ_2 of the effective rate of reaction $\varphi(\vartheta)$, reached at ϑ_1 and ϑ_2 , are equal in accordance with (14) and (15) to the maximum and minimum of the function $\Phi(\theta)$ from (15), obtained with θ_1 and θ_2 , that is,

$$\varphi_{1,2} = \exp \theta_{1,2}, \quad \theta_{1,2} = \theta_{1,3} - \beta \sigma^{-1} \exp \theta_{1,2}, \quad \exp \theta_{1,2} = (\theta_{1,2} - u_m + 1) \beta (\sigma - 1)^{-1}$$

Hence, for example, the result is that when $u_m > \theta$ (Fig. 4) the function $\varphi(\vartheta)$ does not have extreme values.

From Figs. 1 to 4 it follows that in the case $0 \leq u \leq u_m$, i.e., where $0 \leq \vartheta \leq u_m \gamma$, the functions $\theta(\vartheta)$ and $\varphi(\vartheta)$ in (14) are determined for all $0 \leq \gamma \leq 1$. Hence in cases 1, 6, 11, and 12 (Table 1) they are single valued for any γ , and in cases 2 and 10 they are single valued only for $\gamma < \vartheta^{\circ} / u_m$. In the remaining cases the curves $\theta(\vartheta)$ and $\varphi(\vartheta)$ have three branches at certain intervals of variation of ϑ .

In accordance with [7, 9, 11], the steady-state heatings θ of the catalyst surface are stable if $d\theta/d\vartheta > 0$, and unstable if $d\theta/d\vartheta < 0$.

Hence we find that if $u_m < \theta$ (Figs. 1 and 3), then one branch $\theta(\vartheta)$ and, consequently, also $\varphi(\vartheta)$ are always stable, and of the three only two are stable: the first below (ϑ_K) corresponds to the kinetic conditions

in which θ and ϑ are close to each other, and the other (φ_d) corresponds to diffusion conditions, accompanied by strong heating θ of the catalyst (if $\theta < u_m$, we will call them lower diffusion conditions, and if $\theta > u_m$, we will call them upper diffusion conditions).

If $u_m > \theta$ (Figs. 2 and 4), then of the three branches only one is stable: the kinetic branch in cases 7 and 8 and the upper diffusion branch in cases 8-10. One branch is always unstable (cases 11 and 12).

Thus in cases 11 and 12 there is not one stable steady-state condition in the reactors examined.

For each steady state, θ (ϑ) has a fully determined value, and therefore in accordance with the preceding, θ (ϑ) and consequently φ (ϑ) in (14) also are represented here as single-valued, bounded, smooth or piecewise-smooth functions with discontinuities of the first kind (corresponding to the possible change-over of θ (ϑ) at certain sections of the variation of ϑ from one of the existing branches to the other).

It can be shown that in the case of any function $\psi(u\gamma, v\gamma) > 0$ of the type indicated above, which is determined over a corresponding interval, there exists a single solution of the inverse problem (14) and (16) for the case in which γ (i.e., the maximum temperature in the layer or the finite concentration) is given and the length of the layer l is determined (for $\gamma=1$, additional requirements are applied, which, in the case $\lambda=1$, when $\psi=\varphi(u\gamma)$, are reduced to $\varphi(u_m)=0$, $\varphi'(u_m)<0$). For the smooth function $\psi(u\gamma, v\gamma)$ this was shown in [5].

In the case of continuous variation of γ , the values $l(\gamma)$ vary continuously, and, if $\psi(u\gamma, v\gamma)$ is determined for any $0 \leq \gamma \leq 1$, then with variation of γ from 0 to 1 the value of $l(\gamma)$ covers the whole interval $[0, \infty]$. Consequently, the solution of the straight problem (l is given, γ is determined) always exists, i.e., in reactors of arbitrary length at least one steady state is possible. If $\psi(u\gamma, v\gamma)$ is determined, for example, only in the case of $0 \leq \gamma \leq \gamma_1$, then the corresponding conditions exist only in the case $l < l_1$, where $l_1 = \max l(\gamma)$ for $0 \leq \gamma \leq \gamma_1$.

As a result we find that in case 1, in reactors of arbitrary length l , only kinetic systems in which the catalyst temperature θ and the temperature of the flow ϑ are close to each other are realized. These conditions, which are usually low-temperature conditions, are used more often in chemical technology.

In case 5 the kinetic conditions also exist at any l . Together with these, in the case $l < l^{**}$ (a) upper diffusion conditions are also possible; these are accompanied by very strong heating ($\theta > u_m$) of the catalyst ($l^{**} = \max l(\gamma)$ when $0 < \gamma < \vartheta^{**}/u_m$, $\varphi = \varphi_d(u\gamma)$). Moreover, there are still infinitely many mixed steady states, in which case, in the section $0 < \vartheta < \vartheta^{**}$ along the layer of the catalyst, the kinetic conditions alternate with the upper diffusion conditions. In other words in this case, in realizing kinetic conditions there is the danger of ignition of separate parts of the catalyst (owing to random disturbances). In realizing the upper diffusion conditions, there is, correspondingly, a danger of extinction. This is confirmed by the numerical calculations carried out in [13].

In cases 2-4, 7, and 8 the kinetic conditions exist only in reactors whose length is $l < l^*$ (a) ($l^* = \max l(\gamma) > l(\vartheta^*/u_m)$ when $0 < \gamma < \vartheta^*/u_m$, $\varphi = \varphi_k(u\gamma)$). Hence in case 7 there are no other conditions, and in the case $l > l^*$ the steady-state conditions are generally impossible (without calculating they are known to be unstable), and explosion takes place. In case 8, as distinct from case 7, when $a > a^{**}(l)$ and $l^o(a) < l < l^{**}(a)$ upper diffusion conditions are still possible (a^{**}, l^o are certain values which can be determined). In case 3, lower diffusion conditions are still possible together with kinetic conditions (when $l < l^*$) in reactors of arbitrary length l ; under these diffusion conditions there is considerable heating of the catalyst, but it does not exceed the adiabatic heating of the reacting mixture in the case of complete conversion ($\theta_0^o < \theta < u_m$). These are also mixed steady states in which the above-mentioned conditions alternate on the corresponding parts of the catalyst. Case 2 differs from case 3 in that here there are the kind of $l^o(a)$ and $a^*(l)$ values for which only kinetic conditions are possible when $l < l^o$ but for which only mixed conditions are possible when $l \geq l^o$, $a < a^*$. In case 4, as distinct from case 2, there are also upper diffusion conditions together with kinetic conditions when $l < l^{**}$. (It can be shown that lower diffusion conditions are absent when $l < l^{**}$.) The possibility of mixed states with changeover to the upper diffusion condition also appears.

In case 6 there are only lower diffusion conditions in reactors of arbitrary length.

In case 9 the steady-state conditions, which are upper diffusion conditions here, are possible only in reactors of length $l < l^{**}$, and in case 10 they are only possible if $a > a^{**}$ and $l^o < l < l^{**}$.

On the basis of Table 1 and taking into account (18), (24)-(26), (12), and (6), it is possible, in particular, to evaluate the limits up to which either the concentration C_- of the determining reagent in the initial

flow must be reduced, the effective coefficients β_1 and α_1 of the heat and mass transfer from the surface of the grains must be increased (for example, by turbulence of the flow), or the activity of the catalyst (k_0) must be reduced, so that in the examined system only kinetic systems are realized. (In the first case the value u_m is reduced, but in the second and third cases A , θ , $B_{1,2}$ are increased.)

We will also note that the values θ^* and ϑ^* , for example, can be described here as ignition temperatures of the catalyst, since these are maximum temperatures which can be reached by the catalyst and the flow, respectively, in the case of a kinetic condition. In the case of higher temperature values, either only diffusion conditions can be realized (cases 2-4) accompanied by considerably greater heating ignition of the catalyst ($\theta > \theta^*$, where $\theta^* > \theta^*$) or, in general, steady-state conditions become impossible (case 7) and explosion takes place (unlimited increase of θ). The values θ^* and ϑ^* in cases 2 and 4 can be described correspondingly as the extinction temperatures of the catalyst.

If $\lambda \neq 1$, then by using the inequalities (13) it is possible to obtain upper and lower estimates for the existence of different conditions.

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