## STEADY STATES OF A CONTINUOUS-FLOW ADIABATIC CHEMICAL REACTOR

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Flow reactors are widely used in the chemical industry for purposes of catalytic reactions $[1,2]$. Calculation of reactors of this type, even in one-dimensional approximation, is complicated and possible only with the use of numerical methods [1,3]. Such calculations make it possible to find the steady-state distribution of temperature and concentration in the chemical reactor if one exists; in general, however, there may be other steady-state regimes which may be preferable from the standpoint of obtaining a different degree of conversion of the starting product, operating stability, etc.

In this connection special interest attaches to the question of the existence and number of steady-state solutions of the system of equations describing the reactor process.

This problem was previously considered in [4-7]. Thus, in [4,5] it was pointed out that in certain special cases more than one steadystate regime may exist. In $[6,7]$ the question of sufficient conditions of uniqueness was investigated. In [7] it was shown that the steadystate regime is unique in the case of short reactors or a dilute mixture of reactants. In [8] the problem of the existence and uniqueness of the steady-state regime was examined for a chain reaction model with direct application of the general theorems of functional analysis.

The present paper includes an analysis of a very simple mathematical model of an adiabatic chemical reactor in which an exothermic or endothermic reaction takes place. It is established that in the case of an endothermic process a unique steady-state regime always


Fig. 1
exists. In the exothermic case the problem of the steady-state regime also always has a solution which, however, may be nonunique; the possibility of the existence of several steady-state regimes, associated with the form of the temperature dependence of the heat release rate, is substantiated.
§1. Formulation of the problem. Given a number of simplifying assumptions the steady-state processes of heat and mass transfer in a flow reactor can be described by a system of equations of diffusion and heat conduction in the form [1]:

$$
\begin{align*}
& \rho D \frac{d^{2} \xi}{d^{\prime} x^{2}}-m \frac{d \xi}{d x}+\rho r(\xi, T)=0  \tag{1.1}\\
& \frac{x}{c} \frac{d^{2} T}{d x^{2}}-m \frac{d T}{d x}+\frac{h}{c} r(\xi, T)=0 \tag{1.2}
\end{align*}
$$

It is assumed that the reactor is a cylindrical vessel with impermeable and non-heat-conducting lateral surfaces. All the parameters are averaged over the reactor cross section (one-dimensional problem). The reactor is filled with a porous catalytic medium in which the reaction takes place; $\xi$ is the yield or extent of the reaction in moles per unit volume, $T$ is
temperature. The diffusion and heat conduction processes in the reactor are characterized by the effective longitudinal diffusion coefficient $D$ and thermal conductivity, the diffusion coefficients being the same for all the substances participating in the reaction; $\mathrm{m}=\rho \mathrm{u}$, where $\rho$ is the local density of the mixture of


Fig. 2
reactants and reaction products, and $u$ is the filtration rate. The specific heat c takes into account the presence of the catalyst. The function $r(\xi, T)$ describes the relation between the local reaction rate in moles per unit volume per unit time, temperature and yield; $h$ is the heat of reaction (when $h>0$ the reaction is exothermic; when $h<0$, endothermic).

Let the reactor (zone occupied by catalyst) occupy a region $0 \leq x \leq l$. We will consider the case when the regions "before" and "after" the reactor-catalyst bed-are "empty" volumes free of catalyst extending indefinitely into the regions $-\infty<\mathrm{x}<0$ and $l<\mathrm{x}<\infty$ and having cross sections equal to the cross section of the catalyst zone. In this case the boundary conditions for Eqs. (1.1) and (1.2) are easily obtained by considering Eqs. (1.1) and (1.2) in the empty volumes (where the reaction rate is zero, and the transport coefficients and specific heat have corresponding


Fig. 3
values, generally speaking, different from $D, \alpha$, and c) and substituting the conditions of continuity of concentrations, temperature, and diffusion and heat fluxes at the reactor inlet and outlet $[9,10]$. We obtain

$$
\begin{equation*}
-\rho D \frac{d \xi}{d x}+m \xi=0, \quad x=0 ; \quad \frac{d \xi}{d x}=0, \quad x=l \tag{1.3}
\end{equation*}
$$

$$
\begin{equation*}
-\frac{x}{c} \frac{d T}{d x}+m T=m T_{0}, \quad x=0 ; \quad \frac{d T}{d x}=0, \quad x=l \tag{1.4}
\end{equation*}
$$

Here, $\mathrm{T}_{0}$ is the temperature of the starting mixture. We assume that

$$
\begin{equation*}
x / c=\rho D, \quad \text { or } \quad \chi \equiv x / \rho c=D . \tag{1.5}
\end{equation*}
$$

Using (1.5), from (1.1) and (1.2) we obtain the equation

$$
\left(\rho \chi \frac{d^{2}}{d x^{2}}-m \frac{d}{d x}\right)\left(T-\frac{h}{\rho c} \xi\right)=0
$$

integration of which with allowance for boundary conditions (1.3) and (1.4) gives

$$
\begin{equation*}
T(x)-\frac{h}{p c} \xi(x)=T_{0} . \tag{1.6}
\end{equation*}
$$

Equation (1.6) establishes a one-to-one correspondence between the reaction yield and temperature


Fig. 4
at any section of the reactor (similarity of the yield and temperature fields). In this case

$$
r(\xi, T)=r\left(\rho c\left(T_{0}-T\right) / h, T\right)=\Phi(T) .
$$

Consequently, when (1.5) is satisfied, to solve the problem it is sufficient to consider only (1.2) with boundary conditions (1.4) for the temperature.

In the general case the function $\Phi(T)$ is nonlinear; therefore, generally speaking, the problem (1.2), (1.4) does not have an analytic solution. The temperature and concentration distributions can be found only by using approximate methods or numerical integration. We will consider the problem of the existence and number of solutions. First, we will investigate the general form of the function $\Phi(T)$.

The classical expression for the rate of an irreversible chemical reaction when the starting mixture is stoichiometric has the form

$$
\begin{equation*}
r=k_{0} \exp \left(-\frac{E}{R T}\right)\left(\xi_{m}-\xi\right)^{\beta} . \tag{1.7}
\end{equation*}
$$

Here, $k_{0}$ is the preexponential or frequency factor, $E$ is the activation energy, $R$ is the universal gas constant and $\beta$ is the total order of the reaction. The quantity $\xi_{\mathrm{m}}$ is the maximum yield of the reaction corresponding to total conversion of the starting substances into reaction products.

With similarity between the reaction yield and the temperature fields, in accordance with (1.6) the maximum yield $\xi_{\mathrm{m}}$ corresponds to the temperature

$$
T_{m}=T_{0}+\frac{h}{\rho c} \xi_{m}
$$

In the event of an exothermic reaction, $\mathrm{T}_{\mathrm{m}}$ is the maximum possible temperature, and in the event of an endothermic reaction the minimum possible temperature (in the latter case it is assumed that the initial temperature $\mathrm{T}_{0}$ is sufficiently high). However, the value of $\mathrm{T}_{\mathrm{m}}$, like $\xi_{\mathrm{m}}$, cannot be reached in a reactor of finite length (see below); therefore

$$
\begin{align*}
& T_{0} \leqslant T<T_{m} \text { (exothermic reaction) }  \tag{1.8}\\
& T_{m}<T \leqslant T_{0} \text { (endothermic reaction). } \tag{1.9}
\end{align*}
$$

Starting from (1.6)-(1.9) we can draw the following qualitative conclusions relating to the behavior of the function $\Phi(T)$ :

1) the function $\Phi(T)>0$ at all permissible values of $T$ satisfying inequalities (1.8) or (1.9);
2) the function $\Phi\left(\mathrm{T}_{\mathrm{m}}\right)=0$;
3) in the case of an exothermic reaction $\Phi(T)$ at first increases monotonically with increase in T , reaches a maximum, and thendecreases monotonically;
4) in the case of an endothermic reaction $\Phi(T)$ increases monotonically.

We note that the dependence of reaction rate on yield and temperature may have a form different from (1.7). However, the properties of the function $\Phi(T)$ : enumerated above clearly remain unchanged for a broad class of chemical reactions.

For convenience, we will unify the formulation of the problem for exothermic and endothermic reactions. We take the freestream temperature $\mathrm{T}_{0}$ as a reference value and introduce the variable

$$
\theta=\left|T-T_{0}\right|= \begin{cases}T-T_{0} & \text { (exothermic reaction) }  \tag{1.10}\\ T_{0}-T & \text { (endothermic reaction) }\end{cases}
$$

and the function

$$
\begin{equation*}
F(\theta)=\frac{|h|}{\rho c \chi} \Phi\left(T_{0} \pm \theta\right) \tag{1.11}
\end{equation*}
$$

Here, a plus sign is taken in the case of an exothermic, and a minus sign in the case of an endother-


Fig. 5
mic reaction. Using (1.10) and (1.11), we write the problem (1.2), (1.4) in the following form:

$$
\begin{gather*}
d^{2} \theta / d x^{2}-U \frac{d \theta}{d x}+F(\theta)=0, \quad 0 \leqslant \theta \leqslant \theta_{m},  \tag{1.12}\\
d \theta / d x-U \theta=0, \quad x=0 ; \quad d \theta / d x=0, \quad x=1 \\
\left(U=m(\rho x)^{-1}, \quad \theta_{m}=\left|T_{m}-T_{0}\right|\right) . \tag{1.13}
\end{gather*}
$$

It follows from (1.11) and (1.8), (1.9) that the basic properties of the function $F(\theta)$ are the same as those
of the function $\Phi(T)$, except that in the case of an endothermic reaction the monotonic increase of $\Phi(\mathrm{T})$ corresponds to a monotonic decrease of $\mathbf{F}(\theta)$. The general behavior of the function $F(\theta)$ is illustrated in Fig. 1 for exothermic (a) and endothermic (b) reactions.
§2. Existence of steady-state regime. We will first show that the function $\theta(x)$, the solution of the problem (1.12), (1.13), increases monotonically provided that $F(\theta)>0$. With this in mind we multiply Eq. (1.12) by $\exp (-U x)$ and integrate with respect to $x$ from $x$ to $l$. Using the second of conditions (1.1.3), we have

$$
\begin{equation*}
\frac{d \theta}{d x}=e^{U x} \int_{x}^{l} e^{-U x} F(\theta) d x \tag{2.1}
\end{equation*}
$$

It follows from (2.1) that $d \theta / \mathrm{dx}>0$ at $0 \leq x<l$.
In view of the monotonic behavior of the function $\theta(x)$ there is a one-to-one correspondence between $\theta$ and $x\left(0 \leq \theta \leq \theta_{\mathrm{m}}, 0 \leq \mathrm{x} \leq l\right)$. We introduce the function $p(\theta)=d \theta / d x$ and formulate the problem (1.12), (1.13) for the function $p(\theta)$. We have

$$
\begin{gather*}
p \frac{d p}{d \theta}-U p+F(\theta)=0,  \tag{2.2}\\
p=0, \quad \theta=\theta_{f} \quad\left(\theta(l)=\theta_{f}\right),  \tag{2.3}\\
p=U \theta_{i}, \quad \theta=\theta_{i} \quad\left(\theta(0)=\theta_{i}\right) . \tag{2.4}
\end{gather*}
$$

In problem (2.2)-(2.4) the quantities $\theta_{f}$ and $\theta_{i}$ are not given and must be determined in the process of solution.

We provisionally fix $\theta_{f}$. Then problem (2.2), (2.3) is the Cauchy problem. Its solution always exists and is unique. Taking $\theta_{f}$ as parameter, we write this solution in the form $p=p\left(\theta_{f}, \theta_{f}\right)$.

We express the temperature at the reactor inlet in terms of the outlet temperature. The corresponding relation between $\theta_{i}$ and $\theta_{f}$ follows from boundary conditions (2.4) and has the form

$$
p\left(\theta_{i}, \theta_{f}\right)-U \theta_{i}=0
$$

The value of $\theta_{f}$ is found from the condition

$$
\begin{equation*}
l=\int_{\theta_{i}\left(\theta_{f}\right)}^{\theta_{f}} \frac{d \theta}{p\left(\theta_{,} \theta_{f}\right)} \tag{2.5}
\end{equation*}
$$

Condition (2.5) selects the desired solutions of problem (1.12), (1.13) among the set of solutions of problem (2.2)-(2.4).

The temperature distribution in the reactor is determined from the implicit expression

$$
\begin{equation*}
x \div \int_{\theta}^{\theta_{f}} \frac{d \theta}{p\left(\theta, \theta_{f}\right)}=i \tag{2.6}
\end{equation*}
$$

Thus, the question of the existence and number of solutions of the problem (1.12), (1.13) reduces to the investigation of the existence and number of solutions of the problem (2.2)-(2.5).

We note that the above arguments leading to the formulation of the problem in the form (2.2)-(2.5) retain their force if we parametrize the solutions of Eq. (2.2) taking as parameter $\theta_{\mathrm{i}}$, i.e., the reactor inlet temperature. In this case the solutions of (2.2) with boundary condition (2.4) have the form $p=p\left(\theta_{1}, \theta\right)$, the relation between $\theta_{i}$ and $\theta_{f}$ follows from boundary condition (2.3), and so on. From the formal standpoint this approach is completely equivalent to that described above; however, parametrization of the solutions using $\theta_{f}$ as parameter is preferable for purposes of analysis. We will consider the problem of the existence of solutions of problem (2.2)-(2.5). For this purpose we investigate the behavior of the integral curves of Eq. (2.2). The field of these integral curves is shown in Fig. 2. The isocline of zero slope is the curve $\mathrm{P}_{0}(\theta)=U^{-1} F(\theta)$ represented by a heavy line in Fig. 2.

Above this line the integral curves have positive slope, below it, negative slope. The curves intersect the straight line $\mathrm{p}=0$ at right
angles. The point $\theta=\theta_{m}, p=0$ is a singular point (if, for example, $\mathrm{F}^{\prime}\left(\theta_{\mathrm{m}}\right) \neq 0$, this is a saddle point). Figure 2 also shows (dashed line) the straight line $\mathrm{p}=\mathrm{U} \theta$, which by virtue of boundary conditon (2.4) must be the termination of the integral curves-solutions of the problem (2.2), (2.3)-leaving points $\theta=\theta_{f}, p=0$ and entering the upper half-plane. From an analysis of the field of directions of the integral curves it follows that from any point in the interval $\left(0, \theta_{\mathrm{m}}\right)$ an integral curve enters the upper half-plane to intersect the straight line $p=U \theta$ at some point with abscissa $\theta=\theta_{\mathrm{i}}$. Thus, to each value of $\theta_{f}$ there corresponds a value of $\theta_{\mathrm{i}}$.

At fixed $\theta_{f}$, by virtue of the uniqueness of the solution of problem (2.2), (2.3), there is only one integral curve passing through the point $\theta=\theta_{f}, p=0$; consequently, to each value of $\theta_{f}$ there comesponds a unique value of $\theta_{i}$. Clearly, not every integral curve of this type defines a desired solution of the problem (1.12), (1.13), since if $\theta_{f}$ is arbitrarily assigned the solution $p\left(\theta, \theta_{f}\right)$ may not satisfy integral condition (2.5),

We will now consider condition (2.5), which associates a value of $l$ with each value of $\theta_{f}$ and hence determines the function $l\left(\theta_{f}\right)$. It is easy to see that the function $l\left(\theta_{f}\right)$ is continuous on the interval $\left(\theta, \theta_{m}\right)$. This follows from the continuity of the function $\theta_{i} \approx \theta_{i}\left(\theta_{f}\right)$ on that interval and the continuity of the function $p^{-1}\left(\theta, \theta_{f}\right)$ at all $\theta \neq \theta_{f}$. In fact, at $\theta=\theta_{f}$ the function $p^{-1}\left(\theta_{2} \theta_{f}\right)$ has a singularity; however, it can be shown that this singularity is integrable if $\theta_{f} \neq \theta_{\mathrm{m}}$. Actually, it follows from (2.2), (2.3) that the point $\theta=\theta_{f}$ is an algebraic moving critical point of the integral of Eq. (2.2) satisfying condition (2.3), the solution of problem (2.2), (2.3) in a neighborhood of that point having the form

$$
\begin{align*}
& p\left(\theta, \theta_{f}\right)=\sqrt{2 \tilde{F}\left(\theta_{f}\right)}\left(\theta_{f}-\theta\right)^{1 / 2}- \\
& -3 / 3 U\left(\theta_{f}-\theta\right)+0\left(\left(\theta_{f}-\theta\right)^{3 / 2}\right) . \tag{2.7}
\end{align*}
$$

We will now examine the behavior of the function $l\left(\theta_{f}\right)$ as $\theta_{f} \rightarrow$ $\rightarrow 0$ and $\theta_{f} \rightarrow \theta_{\mathrm{m}}$. From an analysis of the integral curve field it follows that as $\theta_{f} \rightarrow 0$ necessarily $\theta_{i} \rightarrow 0$. Therefore, using (2.7), from (2.5) we conclude that

$$
l=2^{1 / 2}\left[F\left(\theta_{j}\right)\right]^{-1 / 2}\left(\theta_{f}-\theta_{i}\right)^{1 / 2}+0\left(\theta_{f}-\theta_{i}\right)
$$

i.e., $l \rightarrow 0$ as $\theta_{f} \rightarrow 0$. Similarly we conclude that $l \rightarrow \infty$ as $\theta_{f} \rightarrow$ $\rightarrow \theta \mathrm{m}$. We note that the latter implies the impossibility of reaching the extremal temperature (maximum in the case of an exothermic reaction and minimum in the case of an endothermic reaction) and hence total conversion of one of the reactants in a reactor of finite length.

It has just been shown that the function $l\left(\theta_{f}\right)$ defined by condition (2.5) is continuous on the interval $\left(\theta, \theta_{\mathrm{m}}\right)$ and takes the values 0 and $\infty$ at the ends of that interval. Hence it follows that with any given value of $l$, where $0<l<\infty$, condition (2.5) associates at least one value of $\theta_{f}$ in the interval $\left(0, \theta_{m}\right)$, i. e., to any reactor length there corresponds at least one value of the outlet temperature. In view of the above reasoning, this implies the existence of a solution of the problem (2.2)-(2.5) and hence of the problem (1.12), (1.13). Thus, steady reactor states always exist irrespective of the type of reaction (exothermic or endothermic).
\$3. Endothermic reaction. Uniqueness of steady-state regime. As already noted, to any value $\theta_{f}\left(0<\theta_{f}<\theta_{\mathrm{m}}\right)$ on the $\theta_{\text {p plane there }}$ uniquely corresponds an integral curve $p\left(\theta, \theta_{f}\right)$. The point of intersection of this curve and initial straight line $p=U \theta$ has the coordinates $\theta=\theta_{\mathrm{i}}, \mathrm{p}=\mathrm{U} \theta_{\mathrm{i}}$. For each $\theta_{f}$ Eq. (2.3) enables us to calculate a value of $l$ and hence determines the function $l\left(\theta_{f}\right)$ or the inverse function $\theta_{f}(U)$.

Obviously, if as $l$ varies on the interval $(0, \infty)$ the function $\theta_{f}(l)$ is unique, then to any value of $l$ there correspond unique values of $\theta_{f}, \theta_{i}$ and a single function $p\left(\theta, \theta_{f}\right)$ satisfying the problem (2.2)-(2.5). In this case the problem of the operating regime of the chemical reactor has a unique solution. However, if the function $\theta_{f}(l)$ is such that to any value $l=l_{*}$ there correspond several values of $\theta_{f}$, the problem of the operating regime of a chemical reactor of length $l$, has several
solutions and the number of solutions is equal to the number of values of $\theta_{f}$ corresponding to the given $l_{*}$. The situation described is illustrated in Fig. 3, where the continuous curve corresponds to the case of a unique solution and the broken line to the case of three solutions at $l=l_{\text {. }}$.

Using Eq. (2.2), we write (2.5) in the form:

$$
l\left(\theta_{f}\right)=\int_{\theta_{i}\left(\theta_{f}\right)}^{\theta_{f}} \frac{U}{F(\theta)} d \theta-\int_{\theta_{i}\left(\theta_{f}\right)}^{\theta_{f}} \frac{1}{F(\theta)} \frac{d p}{d \theta} d \theta .
$$

Then, integrating by parts, and using conditions (2.3), (2.4), we obtain

$$
\begin{align*}
l\left(\theta_{f}\right) & =\int_{\theta_{i}\left(\theta_{f}\right)}^{\theta_{f}} \frac{U}{F(\theta)} d \theta+\frac{U \theta_{i}}{F\left(\theta_{i}\right)}+ \\
& +\int_{\theta_{i}\left(\theta_{f}\right)}^{\theta_{f}} p(\theta) \frac{d}{d \theta}\left(\frac{1}{F(\theta)}\right) d \theta \tag{3.1}
\end{align*}
$$

We find the derivative of the function $l\left(\theta_{f}\right)$. Differentiating (3.1), we obtain

$$
\begin{equation*}
\frac{d l}{d \theta_{f}}=\frac{U}{F\left(\theta_{f}\right)}+\int_{\boldsymbol{\theta}_{i}\left(\theta_{j}\right)}^{\theta_{f}} \frac{d}{d \theta}\left(\frac{1}{F(\theta)}\right) \frac{\partial p}{\partial \theta_{f}} d \theta \tag{3.2}
\end{equation*}
$$

If the right side of (3.2) takes positive values at all permissible values of $\theta_{f}$, the function $l\left(\theta_{f}\right)$ is monotonic and, consequently, the solution of the problem is unique. Thus, the question of the uniqueness of the solution of problem (2.2)-(2.5) can be solved by investigating the sign of the right side of expression (3.2).

In the case of an endothermic reaction the function $F(\theta)$ decreases monotonically. Therefore the first factor in the integrand in (3.2) takes only positive values on the entire interval of integration. We will establish the sign of the second factor. Differentiating Eq. (2.2) with respect to $\theta_{f}$, we find

$$
\begin{equation*}
\frac{d}{d \theta}\left(\frac{\partial p}{\partial \theta_{f}}\right)=\frac{F(\theta)}{p^{2}} \frac{\partial p}{\partial \theta_{j}} . \tag{3.3}
\end{equation*}
$$

We integrate Eq. (3.3) with respect to $\theta$, assuming that $F(\theta)$ and $p=p\left(\theta, \theta_{f}\right)$ are known functions and having determined the constant of integration from the value of the derivative $\partial_{p} / \partial \theta_{f}$, at some point, for example, the point $\theta=\theta_{i}$, we obtain

$$
\begin{equation*}
\frac{\partial p}{\partial \theta_{f}}=\left(\frac{\partial p}{\partial \theta_{f}}\right)_{\theta=\theta_{i}} \exp \left\{-\int_{\theta_{i}}^{\theta} \frac{F}{p^{2}} d \theta\right\} \tag{3.4}
\end{equation*}
$$

From (3.4) it follows that if the derivative $\partial p / \partial \theta_{f}$ at the point $\theta=\theta_{\mathbf{i}}$ is a positive quantity, this derivative retains its positive value over the entire interval in question. As already noted, the constant of integration can be determined from the value of the derivative $\partial p / \partial \theta_{f}$ at any point on the interval $\left[\theta_{i}, \theta_{f}\right]$; therefore, positiveness on the entire interval follows from the positiveness of $\partial \mathrm{p} / \partial \theta_{f}$ at any individual point within that range.

An analysis of the field of integral curves shows that as $\theta_{f}$ increases the integral curves in the $p$, $\theta$ plane corresponding to a larger $\theta_{f}$ pass above the integral curves corresponding to smaller values of $\theta_{f}$. This means that at given $\theta$ the quantity $p\left(\theta_{i} \theta_{f}\right)$ increases with increase in $\theta_{f}$, i.e. , $\partial \mathrm{p} / \partial \theta_{f}>0$.

For the sake of clarity, Fig. 4 gives a qualitative picture of the function $p\left(\theta_{i}, \theta\right)$ representing the surface above the plane $\theta, \theta_{i}$.

Thus, both factors in the integrand on the right side of (3.2) take only positive values, so that in the case of an endothermic reaction the inequality

$$
\begin{equation*}
d l / d \theta_{f}>0 \tag{3.5}
\end{equation*}
$$

is satisfied at any permissible values of $\theta_{f}$.
Consequently, the function $l\left(\theta_{f}\right)$ is monotonic, and the problem of the steady-state operating regime of an endothermic reactor has a unique solution.
§4. Exothermic reaction: In the case of an exothermic reaction the function $F(\theta)$ is nonmonotonic, at a certain value $\theta=\theta^{*}$ it reaches a maximum (Fig. 1a).

In 52 it was shown that if the entire region of permissible temperatures, i.e., the interval $0<\theta<\theta_{\mathrm{m}}$, is considered, a steady-state regime always exists. We will show that: 1) on the interval $0<\theta<\theta^{*}$, where the function $F(\theta)$ increases, a steady-state regime may be lacking, if the function $F(\theta)$ grows sufficiently rapidly; 2) over the entire region of permissible values of the temperature $0<\theta<\theta_{\mathrm{m}}$ the problem may have more than one solution.

We will consider the representation of problem (1.12), (1.13) in the form of an integral equation. To this end we return to Eq. (2.1) and integrate it with respect to $x$, using the first of conditions (1.13). We obtain

$$
\begin{equation*}
\theta=\frac{1}{U} \int_{0}^{1} F(\theta) e^{-U x} d x+\int_{0}^{x} e^{U x} \int_{x}^{l} F(\theta) e^{-U x} d x d x \tag{4.1}
\end{equation*}
$$

In Eq. (4.1) the first term corresponds to the value of the reactor inlet temperature.

Since the function $\theta(x)$ increases monotonically (see §2), we have $\min \theta(x)=\theta(0)=\theta_{\mathrm{i}}$. Then on the interval $\left[0, \theta^{*}\right]$, in view of the growth of the function $F(\theta)$, from (4.1) we have

$$
\begin{equation*}
\theta_{i}>\frac{1-\exp (-U l)}{U^{2}} F\left(\theta_{i}\right) \tag{4.2}
\end{equation*}
$$

We will consider the functions $F(\theta)$ satisfying the condition

$$
\begin{equation*}
\partial F(\theta) / \partial \theta \geqslant K, \quad K>0 \tag{4.3}
\end{equation*}
$$

From (4.3) and the positiveness of $F(\theta)$ it follows that $K \theta_{i} \leq F\left(\theta_{i}\right)$ and from inequality (4.2) that problem (1.12), (1.13) does not have solutions at

$$
\begin{equation*}
l \geqslant \frac{\ln \left(1-U^{2} / K\right)}{U} \tag{4.4}
\end{equation*}
$$

Condition (4.4) means that there is no solution at sufficiently small U and sufficiently large $l$ (see Fig. 5 , where the region of absence of solutions on the plane $l, \mathrm{U}$ is shaded). The physical significance of this is obvious: for small velocities and a long reactor with a highenergy exothermic reaction and no heat losses through the side walls it is not possible for all the heat to be removed through the front ( $x=$ $=0$ ) and rear ( $x=l$ ) ends of the reactor and the temperature rises sharply (analogy with thermal explosion).

We will now consider the question of the number of steady-state reactor regimes for the entire interval $0<\theta<\theta_{\mathrm{m}}$. We return to the analysis of the function $l\left(\theta_{f}\right)$ began in $\S 3$. In this case the function $F(\theta)$ decreases monotonically; therefore the second term on the right side of (3.2) may take negative values. Since on the entire interval of variation of $\theta_{f}$ the function $l\left(\theta_{f}\right)$ varies from 0 (at $\theta_{f}=0$ ) to $\infty$ at $\left(\theta_{f}=\theta_{m}\right.$ ), there follows the possibility of a nonmonotonic variation of the function $l\left(\theta_{f}\right)$. If the function $l\left(\theta_{f}\right)$ is nonmonotonic, certain values of $l_{*}$ may correspond to several values of $\theta_{f}$ and, consequently, problem (2.2)-(2.5) will have several solutions at those values of $l_{*}$.

The number of solutions is determined by the number of points of intersection of the straight line $l=l_{*}$ and the curve $l\left(\theta_{f}\right)$ (see Fig. 3) and must be odd. The nonuniqueness of the solution, i.e., the presence of intervals on which the function $l\left(\theta_{f}\right)$ decreases, is associated with the form of the function $F(\theta)$.

In the plane $\theta$, $p$ we will consider two solutions of problem (2.2), (2.3) corresponding to two different values of $\theta_{f}$ equal to $\theta_{f}^{(1)}$ and $\theta_{f}$, where $\theta_{f}^{(1)}<\theta_{f}$. To each solution there corresponds a value of $\theta_{i}$, which we will denote by $\theta_{i}(\mathbb{I})$ and $\theta_{i}$, respectively. Applying (2.5) to
each of the solutions, we obtain

$$
\begin{align*}
l-l^{(1)} & =\int_{\theta_{i}}^{\theta_{f}^{(1)}}\left[\frac{1}{p\left(\theta_{i}^{(1)}, \theta\right)}-\frac{1}{p\left(\theta_{i}, \theta\right)}\right] d \theta- \\
& -\int_{\substack{0 \\
\theta_{i}^{(1)}}}^{\theta_{i}} \frac{d \theta}{p\left(\theta_{i}^{(1)}, \theta\right)}+\int_{\theta_{i}^{(1)}}^{1} \frac{d \theta}{p\left(\theta_{i}, \theta\right)} . \tag{4.5}
\end{align*}
$$

The inequality

$$
\begin{equation*}
p\left(\theta_{i}, \theta\right)>p\left(\theta_{i}^{(\mathbf{1})}, \theta\right) \tag{4.6}
\end{equation*}
$$

holds for the functions $p\left(\theta_{i}, \theta\right)$ and $p\left(\theta_{i}^{(1)}, \theta\right)$ on the interval $\theta_{i}<\theta<\theta_{i}^{(1)}$. Moreover,

$$
\begin{equation*}
p\left(\theta_{i}, \theta\right)>0, \quad p\left(\theta_{i}^{(1)}, \theta\right)>0 \tag{4.7}
\end{equation*}
$$

In view of $(4.6)$ and (4.7), the first two terms on the right side of (4.5) have values less than zero, so that their sum is equal to some finite negative number, whereas the third term in (4.5) is equal to a positive number.

At values of $\theta_{f}$ corresponding to the interval of variation of $l$, of which $l\left(\theta_{f}\right)$ is a monotonically increasing function, the sum of the integrals in (4.5) is greater than zero.

At values of $\theta_{f}$ corresponding to the region in which $l\left(\theta_{f}\right)$ is a decreasing function, so that one and the same $l$ corresponds to not less than three solutions of the problem (2.2)-(2.5), the sum of the integrals in (4.5) must be negative.

The behavior of the functions $p\left(\theta_{i}, \theta\right)$ and $p\left(\theta_{i}^{(1)}, \theta\right)$ is determined by the character of the function $F(\theta)$. We will show that the nature of variation of the function $F(\theta)$ on the half-open interval $\theta_{f}{ }^{(1)}<\theta \leqslant \theta_{f}$, may be such that the corresponding value of $l\left(\theta_{f}\right)$ is located on the descending branch of the function $l\left(\theta_{f}\right)$. On the half-open interval in question the function $F(\theta)$ must be such that the last integral on the right side of (4.5) is less than the sum of the moduli of the first two integrals, whose value does not depend on the form of the function $F(\theta)$ at $\theta>\theta_{f}^{(1)}$.

For example, let us take the function $F(\theta)$ at $\theta>\theta_{f}^{(1)}$ in the form

$$
\begin{gather*}
F^{0}(\theta)=1 / 2 a_{0}^{2}+\left(2 a_{0} a_{2}-{ }^{2} / \theta^{2} U^{2}\right)\left(\theta_{f}-\theta\right)- \\
-\frac{2}{3} a_{2} U\left(\theta_{f}-\theta\right)^{3 / 2}+3^{3 / 2} a_{2}^{2}\left(\theta_{f}-\theta\right)^{2}, \\
a_{0}=3 / 2 \tau^{-1 / 2} p_{1}+\tau^{1 / 2}\left(p_{1}^{\prime}+1 / 3 U\right), \\
a_{3}=-1 / 2 \tau^{-3 / 2} p_{1}-\tau^{-1 / 2}\left(p_{1}^{\prime}-1 / 2 U\right),\left.\quad p\left(\theta_{i}, \theta\right)\right|_{\theta=\theta_{i}^{(1)}}=p_{1}, \\
\partial p\left(\theta_{i}, \theta\right) /\left.\partial \theta\right|_{\theta=\theta_{f}^{(1)}}=p_{1}^{\prime}, \quad \tau=\theta_{f}-\theta_{f}^{(1)} . \tag{4.8}
\end{gather*}
$$

The quantity $\theta_{f}$ in (4.8) plays the part of a parameter whose specific value will be determined later.

The solution of Ec. (2.2) with condition (2.3) on the interval $\theta_{f}^{(1)} \leqslant \theta_{f}$, where the function $F(\theta)$ is found from (4.8), has the torm

$$
p^{\circ}(\theta)=a_{0}\left(\theta_{f}-\theta\right)^{1 / 2}-\frac{2}{3} U\left(\theta_{f}-\theta\right)+a_{2}\left(\theta_{f}-\theta\right)^{3 / 2} .
$$

It can be seen that the solution $p^{\circ}(\theta)$ and its derivative are "joined" with the solution $p\left(\theta_{j}, \theta\right)$ at the point $\theta=\theta_{j}^{(1)}$, so that, taken together, the functions $p\left(\theta_{i}, \theta\right)\left(\theta_{i} \leqslant \theta \leqslant \theta_{f}^{(1)}\right), p^{0}(\theta)\left(\theta_{f}^{(1)}<\theta \leqslant \theta_{f}\right)$ will be a solution of the problem (2.2)-(2.4) on the entire interval $\theta_{i} \leq \theta \leq \theta_{f}$ if

$$
F(\theta)=F(\theta), \quad \theta_{i} \leqslant \theta_{f}^{(1)} ; F(\theta)=F^{\circ}(\theta), \quad \theta_{f}^{(1)}<\theta \leqslant \theta_{f} . \quad \text { (4.9) }
$$

In this case the last integral on the right side of (4.5) can be written in the explicit form:

$$
\begin{equation*}
2 \int_{0}^{t_{0}^{1 / 2}} \frac{d t}{a_{0}-2 / 3 t t+a_{2} t^{2}} . \tag{4.10}
\end{equation*}
$$

It follows from (4.8) that by reducing $\theta_{f}$ (and consequently $\tau$ ) we can make the value of the integral (4.10) less than any predetermined
number, i.e., there is always a value $\theta_{f}=\theta_{f}$ such that at $\theta_{f}<\theta_{f}$ the inequality

$$
\begin{align*}
& \int_{\theta_{f}^{(1)}}^{\theta_{f}} \frac{d \theta}{p\left(\theta_{i}, \theta\right)}<\int_{\theta_{i}}^{\theta_{f}^{(1)}}\left[\frac{1}{p\left(\theta_{i}^{(1)}, \theta\right)}-\right. \\
& \left.-\frac{1}{p\left(\theta_{i}, \theta\right)}\right] d \theta+\int_{\theta_{i}^{(1)}}^{\theta_{i}} \frac{d \theta}{p\left(\theta_{i}^{(1)}, \theta\right)} \tag{4.11}
\end{align*}
$$

will be satisfied.
From (4.11), in accordance with (4.5), there follows

$$
\begin{equation*}
l<l^{(1)} \tag{4.12}
\end{equation*}
$$

Thus, if the function $F(\theta)$ has the form (4.9), there are always values of $\theta_{f}$ (we recall that the quantity $\theta_{f}$ enters into the function $\mathrm{F}^{\circ}(\theta)$ as a parameter) at which the solution Eq. (2.2) on the interval $\theta_{j}^{(1)} \leqslant \theta \leqslant \theta_{f}$, joined by the continuous first derivative with the solution of Eq. (2.2) on the interval $\theta_{i} \leqslant \theta \leqslant \theta_{f}^{(1)}$, satisfies inequality (4.11). It can be asserted that to the corresponding value of $l\left(\theta_{f}\right)$ there correspond at least three solutions of the problem (2.2)-(2.5).

We note that the approximation of the function $F^{\circ}(\theta)$ is not too artificial. True, at the point $\theta=\theta_{j}^{(1)}$ the function $F^{\circ}(\theta)$ is "joined" with the function $F(\theta)$ with a discontinuity of the first derivative. Ob wiously, a smooth joint at that point cannot seriously affect the value of the integral (4.10) and hence inequality (4.12).

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