STABILITY OF A POLYTROPIC CHEMICAL REACTOR

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The stability of the steady states of a flow-type chemical reactor has been analyzed previously in [1]. The adiabatic conditions of the process made it possible to reduce the system of two partial differential equations for temperature and concentration to one equation for temperature. In the general case, with allowance for heat losses, which always occur in actual objects, the problem remains essentially two-dimensional, and this leads to a qualitatively new result: bifurcation of steady solutions gives rise to solutions that are periodic in time. The qualitative difference between the solutions of the adiabatic and polytropic problems remains in the case of an ideal-mixing reactor [2]. Indeed, bifurcation of a steady state to a periodic-in-time flow is typical of many-dimensional problems formulated as systems of both ordinary differential equations and partial differential equations. In this case, a one-dimensional (in temperature) nonlinear problem formulated in infinite-dimensional space can have, along with steady solutions, periodic solutions, which result from the secondary bifurcation due to the nonlinearity of the law of heat release. This is the case when the solution of an infinite-dimensional problem is attracted to finite-dimensional space of dimension $\geqslant 2$. If the solution is attracted to two-dimensional space, periodic solutions develop if the double real root of the characteristic cubic equation obtained in [1] splits into a pair of complex conjugate roots. The stability conditions for periodic-in-time solutions that result from secondary bifurcation are presented in [3].

According to the procedure adopted in [1], the stability of a polytropic chemical reactor is studied by the projection method [4], although the problem considered can be reduced to the central variety. The latter method was applied to analysis of the cycle-birth bifurcation in a "brusselator" [5]. The absence of quadratic terms in unknown functions in the nonlinear mathematical model of a "brusselator" simplifies an analysis considerably. However, in spite of this, application of the theorem on the central variety brings about, in our opinion, more cumbersome calculations in comparison with the projection method.

In the statement of the problem, all parameters are initially given in dimensional quantities, and the functions are specified. This is done to narrow the area of stability investigation, which follows from the physical restrictions on the parameters and their functions.

1. The operation of a polytropic chemical reactor is described by the following system of differential equations [6]:

$$\partial T(x_1, t_1)/\partial t_1 = \ae \partial^2 T(x_1, t_1)/\partial x_1^2 - w_1 \partial T(x_1, t_1)/\partial x_1 + Q k_0 c_p^{-1} \varphi(T, c) - \varphi_1(T); \qquad (1.1)$$

$$\partial c(x_1, t_1)/\partial t_1 = D \partial^2 c(x_1, t_1)/\partial x_1^2 - w_1 \partial T(x_1, t_1)/\partial x_1 - k_0 \varphi(T, c). \qquad (1.2)$$

Here x_1 is the coordinate; t_1 is time; T is the temperature; $\ae$ is the thermal diffusivity; c is the concentration; Q is the reaction-heat release per unit mass; E is the activation energy; R is the universal gas constant; k_0 is the preexponential factor; c_p is the specific heat; w_1 is the flow velocity; $\varphi(T, c)$ is a function that characterizes the heat-release intensity in the flow; and $\varphi_1(T)$ is a heat-loss function. Without loss of generality we assume that a reaction of the Langmuir–Hinshelwood type with an Arrhenius heat release rate proceeds in the reactor, and the heat loss is a linear function of temperature: $\varphi(T, c) = k_1 c(x_1, t_1) \exp\left(-E(RT(x_1, t_1))^{-1}\right)(1 + k_2 c(x_1, t_1))^{-2}$ and $\varphi_1(T) = k_3(T(x_1, t_1) - T(0, t_1))$, where k_1, k_2, and k_3 are constants. In addition, we suppose that the mechanisms of conductive heat transfer and material diffusion are the same and, hence, $D \cong \ae$.

The temperature $T(x_1, t_1)$ and the concentration $c(x_1, t_1)$ satisfy the initial and boundary conditions

$$T(x_1, t_{10}) = T_0, \quad c(x_1, t_{10}) = c_0; \tag{1.3}$$

$$T(0, t_1) = T_0, \quad c(0, t_1) = c_0, \quad \partial T(l_1, t_1)/\partial x_1 = 0, \quad \partial c(l_1, t_1)/\partial x_1 = 0, \tag{1.4}$$

where t_{10} is the initial time and l_1 is the reactor length.

For further analysis, we introduce the generally adopted time and length scales: $t_a = c_p R T_0^2 (EQk_0)^{-1} \exp(E(RT_0)^{-1})$, and $x_a = (\mathscr{æ}t_a)^{0.5}$ and, using these scales, define the dimensionless coordinates and parameters: $t = t_1 t_a^{-1}$, $t_0 = t_{10} t_a^{-1}$, $x = x_1 x_a^{-1}$, $l = l_1 x_a^{-1}$, $w = w_1 t_a x_a^{-1}$, $\beta = RT_0^2 E^{-1}$, $\alpha = k_0 t_a c_0^{-1}$, $\alpha_1 = k_3 RT_0^2 E^{-1}$, and

$$\mathbf{U} = \left\| \begin{array}{c} U_1 \\ U_2 \end{array} \right\| = \left\| \begin{array}{c} E(T - T_0)R^{-1}T_0^{-2} \exp(0.5wx) \\ (c - c_0)c_0^{-1} \exp(0.5wx) \end{array} \right\|.$$

Let us write the functions $\varphi(T, c)$ and $\varphi_1(T)$ in the new variables in the form

$$\varphi(U_1, U_2) = c_0 k_1 (1 + U_2 \exp(-0.5wx))(1 + k_2 c_0 (1 + U_2 \exp(-0.5wx)))^{-2}$$

$$\times \exp(U_1 \exp(-0.5wx)(1 + \beta U_1 \exp(-0.5wx))^{-1}),$$

$$\varphi_1(U_1) = \alpha_1 U_1 \exp(-0.5wx).$$

The function $\varphi(U_1, U_2)$ can be represented in the vicinity of the point $\mathbf{U} = 0$ as the series

$$\varphi(U_1, U_2) = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \varphi_{i,j} U_1^i U_2^j \exp(-0.5wx), \quad \varphi_{i,j} = \frac{1}{i!j!} \exp(0.5wx) \partial^{i+j} \varphi(0,0)/\partial U_1^i \partial U_2^j.$$

Having grouped terms with the same degrees of U_1 and U_2, we now write system (1.1) and (1.2) with conditions (1.3) and (1.4) in dimensionless variables:

$$\partial \mathbf{U}/\partial t = \mathbf{AU} + \mathbf{B}(\mathbf{U}, \mathbf{U}) + \mathbf{C}(\mathbf{U}, \mathbf{U}, \mathbf{U}) + \mathbf{\Phi}(0, 0) + O(|\mathbf{U}|^4); \tag{1.5}$$

$$\mathbf{U}(x, t_0) = 0; \tag{1.6}$$

$$\mathbf{U}(0, t) = 0, \quad \frac{\partial \mathbf{U}(l, t)}{\partial x} - 0.5w\mathbf{U}(l, t) = 0. \tag{1.7}$$

Let us represent the constant $\mathbf{\Phi}(0, 0)$, linear $\mathbf{AU}$, and nonlinear $\mathbf{B}(\mathbf{U}, \mathbf{U})$ and $\mathbf{C}(\mathbf{U}, \mathbf{U}, \mathbf{U})$ operators as

$$\mathbf{\Phi}(0, 0) = \left\| \begin{array}{c} \varphi(0, 0) \\ -\alpha\varphi(0, 0) \end{array} \right\|,$$

$$\mathbf{AU} = \left\| \begin{array}{cc} \partial^2/\partial x^2 + \varphi_{1,0} - \alpha_1 - 0.25w^2 & \varphi_{0,1} \\ -\alpha\varphi_{1,0} & \partial^2/\partial x^2 - \alpha\varphi_{0,1} - 0.25w^2 \end{array} \right\| \left\| \begin{array}{c} U_1 \\ U_2 \end{array} \right\|,$$

$$\mathbf{B}(\mathbf{U}, \mathbf{U}) = \left\| \begin{array}{ccc} \varphi_{2,0} & \varphi_{1,1} & \varphi_{0,2} \\ -\alpha\varphi_{2,0} & -\alpha\varphi_{1,1} & -\alpha\varphi_{0,2} \end{array} \right\| \left\| \begin{array}{ccc} U_1^2 & U_1 U_2 & U_2^2 \end{array} \right\|^t,$$

$$\mathbf{C}(\mathbf{U}, \mathbf{U}, \mathbf{U}) = \left\| \begin{array}{cccc} \varphi_{3,0} & \varphi_{2,1} & \varphi_{1,2} & \varphi_{0,3} \\ -\alpha\varphi_{3,0} & -\alpha\varphi_{2,1} & -\alpha\varphi_{1,2} & -\alpha\varphi_{0,3} \end{array} \right\| \left\| \begin{array}{cccc} U_1^3 & U_1^2 U_2 & U_1 U_2^2 & U_2^3 \end{array} \right\|^t,$$

where $\| \cdot \|^t$ is the transpose.

The stability of a solution of Eq. (1.5) with conditions (1.6) and (1.7) can be established after solving the spectral problem

$$\sigma \mathbf{U} = \mathbf{AU}. \tag{1.8}$$

With allowance for (1.6) and(1.7), the solutions of Eq. (1.8) are the eigenvectors

$$\mathbf{y}_n = \left\| \begin{array}{c} a_n \\ b_n \end{array} \right\| \sin(\lambda_n x).$$

Here λ_n are positive roots of the equation $\tan(\lambda l) = 2\lambda w^{-1}$, arranged in ascending order: $\lambda_1 < \lambda_2 < \dots$. The values of a_n and b_n ($n = 1, 2, \dots$) are calculated with accuracy to a constant factor, and the relation between them is found by solution of the equation $(\mathbf{A} - \sigma_n \mathbf{I})\mathbf{U} = 0$, where σ_n is the value of the parameter σ for $\lambda = \lambda_n$ and $\mathbf{I}$ is a 2×2 unit matrix. If we assume that $a_n = 1$, then $b_n = (\lambda_n^2 + 0.25w^2 + \alpha_1 - \varphi_{1,0} - \sigma_n)\varphi_{0,1}^{-1}$ ($n = 1, 2, \dots$).

The spectrum of the operator $\mathbf{A}$ consists exclusively of the discrete eigenvalues σ_n ($n = 1, 2, \dots$) satisfying the equations

$$\sigma_n^2 + \sigma_n(2\lambda_n^2 + 0.5w^2 + \alpha\varphi_{0,1} + \alpha_1 - \varphi_{1,0}) + \alpha\alpha_1\varphi_{0,1} + (\lambda_n^2 + 0.25w^2)(\lambda_n^2 + 0.25w^2 + \alpha\varphi_{0,1} + \alpha_1 - \varphi_{1,0}) = 0. \quad (1.9)$$

Among the real or complex conjugate roots of Eqs. (1.9) there is a pair of roots containing the largest real root or the largest real part. If these roots are real, analysis of the stability of equilibrium states is performed as in [1, 3]. In the case of complex conjugate roots, they have the largest real part for $n = 1$. Then, if $\mathrm{Re}\,\sigma_1 = 0$, the remaining part of the spectrum of the operator $\mathbf{A}$ is in the left-hand side of the complex plane.

The first ($n = 1$) of Eqs. (1.9) has a pair of purely imaginary roots if and only if $\varphi_{1,0} - a = 0$, $\alpha\alpha_1\varphi_{0,1} - (\lambda_1^2 + 0.25w^2)^2 > 0$, where $a = 2\lambda_1^2 + 0.5w^2 + \alpha\varphi_{0,1} + \alpha_1$.

Denoting the real part of the eigenvalue σ_1 multiplied into 2 by $\mu = \mathrm{Re}\,\sigma_1 = 0.5(\varphi_{1,0} - a)$ and defining the frequency at the point $\mu = 0$ as $\omega_0 = \mathrm{Im}\,\sigma_1 = (\alpha\alpha_1\varphi_{0,1} - (\lambda_1^2 + 0.25w^2)^2)^{0.5}$, we conclude that the periodic solution of the equation $\partial\mathbf{U}/\partial t = \mathbf{A}\mathbf{U}$ that has the frequency ω_0 loses its stability rigorously when μ passes, while growing, through the critical point $\mu = 0$.

The eigenvector corresponding to the eigenvalue σ_1 for $\mu = 0$ has the form

$$\mathbf{y}_1 = \left\|\begin{array}{c} 1 \\ (-\eta + i\omega_0)\varphi_{0,1}^{-1} \end{array}\right\| \sin(\lambda_1 x) \qquad (\eta = \lambda_1^2 + \alpha\varphi_{0,1} + 0.25w^2).$$

To analyze the stability of the solution of the nonlinear equation (1.5), we first assume that the defect destroying a bifurcation at the point $\mu = 0$ is equal to zero: $\varphi(0,0) = 0$.

Substitution of $\varphi_{1,0} = 2\mu + a$ into the expression for the operator $\mathbf{A}$ in the vicinity of the point $\mu = 0$ gives the dependence $\mathbf{A} = \mathbf{A}(\mu) = \mathbf{A}(0) + \mu\partial\mathbf{A}(0)/\partial\mu$, which permits rewriting (1.5) with allowance for the adopted assumption $\varphi(0,0) = 0$:

$$\partial\mathbf{U}/\partial t = (\mathbf{A}(0) + \mu\partial\mathbf{A}(0)/\partial\mu)\mathbf{U} + \mathbf{B}(\mathbf{U},\mathbf{U}) + \mathbf{C}(\mathbf{U},\mathbf{U},\mathbf{U}) + O(|\mathbf{U}|^4). \quad (1.10)$$

The linear $\mathbf{A}(0) + \mu\partial\mathbf{A}(0)/\partial\mu$ and nonlinear $\mathbf{B}(\mathbf{U},\mathbf{U})$ and $\mathbf{C}(\mathbf{U},\mathbf{U},\mathbf{U})$ operators are defined in the space of the eigenvectors $\mathbf{y}_n$ ($n = 1, 2, \dots$).

2. At the critical point $\mu = 0$ two periodic-in-time independent solutions $\mathbf{z}_1 = \mathbf{y}_1 \exp(is)$ and $\bar{\mathbf{z}}_1 = \bar{\mathbf{y}}_1 \exp(-is)$ (the over-bar designates complex conjugacy, $s = \omega_0 t$) fork from the solution of the equation $\mathbf{A}\mathbf{U} = 0$. The other solutions ($\mathbf{z}_n$, $\bar{\mathbf{z}}_n$, $n > 1$), which correspond to the eigenvalues σ_n with a negative real part, decrease exponentially with time.

The vectors $\mathbf{z}_1$ and $\bar{\mathbf{z}}_1$ are 2π-periodic functions and belong to the zero space of the operator

$$\mathbf{L}_s = \left\|\begin{array}{cc} -\omega_0\partial/\partial s + \partial^2/\partial x^2 + 2\lambda_1^2 + \alpha\varphi_{0,1} + 0.25w^2 & \varphi_{0,1} \\ -a\alpha & -\omega_0\partial/\partial s + \partial^2/\partial x^2 - \alpha\varphi_{0,1} - 0.25w^2 \end{array}\right\|,$$

which is endowed with a scalar product on the rectangle $(0, l) \times (0, 2\pi)$:

$$\langle \mathbf{z}_m, \mathbf{z}_n \rangle = \frac{1}{2\pi} \int_0^{2\pi} \int_0^l \mathbf{z}_m^t \bar{\mathbf{z}}_n \, dx \, ds.$$

To construct a bifurcation solution of (1.10), we define the amplitude ε as the scalar product $\varepsilon = \langle \mathbf{U}, \mathbf{z}_1^* \rangle$, where $\mathbf{z}_1^*$ is the eigenvector of the conjugate operator

$$\mathbf{L}_s^* = \left\|\begin{array}{cc} \omega_0\partial/\partial s + \partial^2/\partial x^2 + 2\lambda_1^2 + \alpha\varphi_{0,1} + 0.25w^2 & -a\alpha \\ \varphi_{0,1} & \omega_0\partial/\partial s + \partial^2/\partial x^2 - \alpha\varphi_{0,1} - 0.25w^2 \end{array}\right\|,$$

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which acts on arbitrary vectors z_i and z_j so that $\langle L_s z_i, z_j \rangle = \langle z_i, L_s^* z_j \rangle$. Solving the equation $L_s^* U = 0$, we find with accuracy to a constant factor γ that the eigenvalue σ_1 corresponds to the vector $z_1^* = y_1^* \exp(is)$, where

$$y_1^* = \gamma \left\| \begin{array}{c} a\alpha \\ \eta + i\omega_0 \end{array} \right\| \sin(\lambda_1 x).$$

One can easily verify that $\langle z_1, \bar{z}_1^* \rangle = \langle \bar{z}_1, z_1^* \rangle = 0$ and $\langle z_n, z_1^* \rangle = 0$ for $n > 1$.

Now the 2π-periodic solutions $U(s, \varepsilon) = U(s + 2\pi, \varepsilon)$, $\mu(\varepsilon)$, and $\omega(\varepsilon)$ of Eq. (1.10) can be represented as power series in amplitude ε:

$$\begin{bmatrix} U(s,\varepsilon) \\ \mu(\varepsilon) \\ \omega(\varepsilon) - \omega_0 \end{bmatrix} = \sum_{n=1}^{\infty} \frac{\varepsilon^n}{n!} \begin{bmatrix} U_n(s) \\ \mu_n \\ \omega_n \end{bmatrix}. \tag{2.1}$$

Here $U_n(s) = \| U_{1n} \ U_{2n} \|^t$; μ_n and ω_n are functions and coefficients to be determined.

Differentiating the expression

$$\varepsilon = \langle U, z_1^* \rangle = \left\langle \sum_{n=1}^{\infty} \frac{\varepsilon^n}{n!} U_n(s), z_1^* \right\rangle$$

with respect to ε, we find

$$\left\langle \sum_{n=1}^{\infty} \frac{\varepsilon^{n-1}}{(n-1)!} U_n(s), z_1^* \right\rangle = 1.$$

The definition of the amplitude ε remains valid if $\langle U_1(s), z_1^* \rangle = 1$ and $\langle U_n(s), z_1^* \rangle = 0$ for $n > 1$. The normalization condition $\langle U_1(s), z_1^* \rangle = 1$ makes it possible to find the constant

$$\gamma = \frac{\lambda_1 \varphi_{0,1}(\omega_0 - i\eta)}{\omega_0(\omega_0^2 + \eta^2)(\lambda_1 l - \sin(\lambda_1 l)\cos(\lambda_1 l))},$$

and then

$$z_1^* = \frac{\lambda_1 \varphi_{0,1}(\omega_0 - i\eta)\sin(\lambda_1 x)\exp(is)}{\omega_0(\omega_0^2 + \eta^2)(\lambda_1 l - \sin(\lambda_1 l)\cos(\lambda_1 l))} \left\| \begin{array}{c} a\alpha(\omega_0 + i\eta) \\ i(\omega_0^2 + \eta^2) \end{array} \right\|.$$

Substituting series (2.1) into Eq. (1.10) and identifying the terms with independent powers of ε yields a system of equations for the unknown functions $U_n(s)$ and coefficients μ_n and ω_n:

$$L_s U_1 = 0; \tag{2.2}$$

$$L_s U_2 - 2\omega_1 \partial U_1/\partial s + 2\mu_1 \partial A(0)/\partial\mu U_1 + B(U_1, U_1) = 0; \tag{2.3}$$

$$L_s U_3 - 3\omega_1 \partial U_2/\partial s + 3\mu_1 \partial A(0)/\partial\mu U_2 - 3\omega_2 \partial U_1/\partial s + 3\mu_2 \partial A(0)/\partial\mu U_1 \tag{2.4}$$

$$+ B(U_1, U_2) + C(U_1, U_1, U_1) = 0,$$

and for any $n > 3$ we have $L_s U_n - n\omega_{n-1}\partial U_1/\partial s + n\mu_{n-1}\partial A(0)/\partial\mu U_1 - n\omega_1 \partial U_{n-1}/\partial s + n\mu_1 \partial A(0)/\partial\mu U_{n-1} + R_{n-2} = 0$, where R_{n-2} depends on U_k, ω_k, and μ_k $(k < n-1)$.

Any linear combination of the independent vectors z_1 and $\bar{z}_1$ that are made to vanish by the operator L_s can be a solution of Eq. (2.2). The vectors U_n belong to real space, and, therefore, $U_1 = bz_1 + \bar{b}\bar{z}_1$. In determining the constant b we proceed from the fact that the initial time t_0 is not yet established, and is chosen so that the number $b\exp(i\omega_0 t_0)$ is real for $s = \omega_0(t + t_0)$. Then, without loss of generality, we can write $U_1 = b\exp(i\omega_0 t_0)(z_1 + \bar{z}_1)$. Next, taking into account the normalization $\langle U_1, z_1^* \rangle = 1$, we have $b\exp(i\omega_0 t_0) = 1$, $U_1 = z_1 + \bar{z}_1$ or

$$U_1 = 2\sin(\lambda_1 x) \left\| \begin{array}{c} \cos s \\ -\eta \cos s - \omega_0 \sin s \end{array} \right\|.$$

The condition of solvability of Eq. (2.3), which follows from Fredholm's theorem on the alternative, is formulated as $\langle L_s U_2, z_1^* \rangle = 0$, which allows us to obtain one equation in coefficients μ_1 and ω_1 in complex form:

$$2\mu_1 \langle \partial A(0)/\partial \mu U_1, z_1^* \rangle - 2\omega_1 \langle \partial U_1/\partial s, z_1^* \rangle + \langle B(U_1, U_1), z_1^* \rangle = 0. \tag{2.5}$$

Equation (2.5) splits into two equations in real form:

$$2\mu_1 \langle \partial A(0)/\partial \mu U_1, z_1^* \rangle + \text{Re}\langle B(U_1, U_1), z_1^* \rangle = 0,$$

$$-2\omega_1 \text{Im}\langle \partial U_1/\partial s, z_1^* \rangle + \text{Im}\langle B(U_1, U_1), z_1^* \rangle = 0.$$

The real and imaginary parts of the scalar product $\langle B(U_1, U_1), z_1^* \rangle$ vanish on integration over s, and, therefore, taking into account that $\langle U_1, z_1^* \rangle = 1$ and $\langle \partial U_1/\partial s, z_1^* \rangle = i$, we have $\mu_1 = 0$ and $\omega_1 = 0$.

For $\mu_1 = 0$ and $\omega_1 = 0$, the solution of Eq. (2.3) consists of the general solution of the equation $L_s U_2 = 0$ and any particular solution of the inhomogeneous equation

$$L_s U_2 = -B(U_1, U_1). \tag{2.6}$$

At the same time, as was shown above, the condition $\langle U_2, z_1^* \rangle = 0$ must be satisfied. The general solution U_{2g} of the homogeneous equation $L_s U_2 = 0$ can be any linear combination $U_{2g} = \gamma_1 z_1 + \bar{\gamma}_1 \bar{z}_1$ of the vectors z_1 and $\bar{z}_1$, (γ_1 is a constant).

Before obtaining a particular solution U_{2p} of the inhomogeneous equation (2.6), we represent the operator $B(U_1, U_1)$ in the form

$$B(U_1, U_1) = \sin^2(\lambda_1 x) \exp(-0.5wx) \left\| \begin{array}{c} \Delta_{11} \sin^2 s + \Delta_{12} \cos^2 s + \Delta_{13} \sin s \cos s \\ \Delta_{21} \sin^2 s + \Delta_{22} \cos^2 s + \Delta_{23} \sin s \cos s \end{array} \right\|,$$

where $\Delta_{11} = 4\omega_0^2 \varphi_{0,2} \exp(0.5wx)$; $\Delta_{12} = 4(\varphi_{2,0} - \eta\varphi_{1,1} + \eta^2 \varphi_{0,2}) \exp(0.5wx)$; $\Delta_{13} = 4(2\eta\omega_0\varphi_{0,2} - \omega_0\varphi_{1,1}) \exp(0.5wx)$; and $\Delta_{2i} = -\alpha\Delta_{1i}$ ($i = 1$–3). The special form of the right-hand side of (2.6) and the method of separation of variables allow us to seek a particular solution of this equation as

$$U_{2p} = \exp(-0.5wx) \left\| \begin{array}{ccc} N_1 & M_1 & N_2^t \\ N_1 & M_2 & N_2^t \end{array} \right\|, \tag{2.7}$$

where

$$N_1 = \| \sin^2(\lambda_1 x) \quad \cos^2(\lambda_1 x) \quad \sin(\lambda_1 x)\cos(\lambda_1 x) \|; \qquad N_2 = \| \sin^2 s \quad \cos^2 s \quad \sin s \cos s \|;$$

$M_1 = \|a_{ij}\|$, $M_2 = \|b_{ij}\|$ and $(i, j = 1$–3) are matrices of undetermined coefficients.

Substitution of (2.7) into (2.6) yields a system of 18 linear algebraic equations in unknown coefficients a_{ij} and b_{ij} ($i, j = 1$–3).

Thus, the sum $U_2 = U_{2g} + U_{2p}$, in which U_{2g} depends on the constant factor γ_1, is a solution of Eq. (2.3). To determine γ_1, we use the condition $\langle U_2, z_1^* \rangle = \langle U_{2g}, z_1^* \rangle + \langle U_{2p}, z_1^* \rangle = 0$. Since $\langle U_{2p}, z_1^* \rangle$ vanishes upon integration over s, $\langle \bar{z}_1, z_1^* \rangle = 0$ and $\langle z_1, z_1^* \rangle = 1$, this condition is satisfied if $\gamma_1 = 0$ and, consequently, $U_2 = U_{2p}$. It is worth noting that if the function $\varphi(U_1, U_2)$ is not equal identically to zero, i.e., c_0 and k_1 are nonzero, there is no combination of the process parameters such that $U_2 = 0$. Indeed, if $c_0 \neq 0$ and $k_1 \neq 0$, then $\varphi_{1,1} \neq 0$, and the function Δ_{13} equals zero only when $\varphi_{0,2} \neq 0$, but then $\Delta_{11} \neq 0$. Therefore, $B(U_1, U_1) \neq 0$ and $U_2 \neq 0$.

The condition of solvability of Eq. (2.4) $\langle L_s U_3, z_1^* \rangle = 0$ produces one equation in unknown coefficients μ_2 and ω_2 in complex form

$$3\mu_2 \langle \partial A(0)/\partial \mu U_1, z_1^* \rangle - 3\omega_2 \langle \partial U_1/\partial s, z_1^* \rangle + 3\langle B(U_1, U_2), z_1^* \rangle + \langle C(U_1, U_1, U_1), z_1^* \rangle = 0$$

or two equations in real form

$$3\mu_2 \langle \partial A(0)/\partial \mu U_1, z_1^* \rangle + 3\text{Re}\langle B(U_1, U_2), z_1^* \rangle + \text{Re}\langle C(U_1, U_1, U_1), z_1^* \rangle = 0; \tag{2.8}$$

$$-3\omega_2 \text{Im}\langle \partial U_1/\partial s, z_1^* \rangle + 3\text{Im}\langle B(U_1, U_2), z_1^* \rangle + \text{Im}\langle C(U_1, U_1, U_1), z_1^* \rangle = 0. \tag{2.9}$$

The operators $\mathbf{B}(\mathbf{U}_1, \mathbf{U}_2)$ and $\mathbf{C}(\mathbf{U}_1, \mathbf{U}_1, \mathbf{U}_1)$ are defined as

$$\mathbf{B}(\mathbf{U}_1, \mathbf{U}_2) = \left\| \begin{matrix} \varphi_{2,0} & \varphi_{1,1} & \varphi_{0,2} \\ -\alpha\varphi_{2,0} & -\alpha\varphi_{1,1} & -\alpha\varphi_{0,2} \end{matrix} \right\| \, \| 2U_{11}U_{12} \quad U_{12}U_{21} + U_{11}U_{22} \quad 2U_{21}U_{22} \|^t,$$

$$\mathbf{C}(\mathbf{U}_1, \mathbf{U}_1, \mathbf{U}_1) = \left\| \begin{matrix} \varphi_{3,0} & \varphi_{2,1} & \varphi_{1,2} & \varphi_{0,3} \\ -\alpha\varphi_{3,0} & -\alpha\varphi_{2,1} & -\alpha\varphi_{1,2} & -\alpha\varphi_{0,3} \end{matrix} \right\| \, \| U_{11}^3 \quad U_{11}^2 U_{21} \quad U_{11}U_{21}^2 \quad U_{21}^3 \|^t.$$

Taking into account that

$$\langle \partial \mathbf{A}(0)/\partial\mu\mathbf{U}_1, \mathbf{z}_1^* \rangle = 2\langle z_1 + \bar{z}_1, \mathbf{z}_1^* \rangle = 2, \quad \langle \partial \mathbf{U}_1/\partial s, \mathbf{z}_1^* \rangle = \langle iz_1 - i\bar{z}_1, \mathbf{z}_1^* \rangle = i$$

from Eqs. (2.8) and (2.9) we find

$$\mu_2 = -\frac{\operatorname{Re}\left[3\langle \mathbf{B}(\mathbf{U}_1, \mathbf{U}_2), \mathbf{z}_1^* \rangle + \langle \mathbf{C}(\mathbf{U}_1, \mathbf{U}_1, \mathbf{U}_1), \mathbf{z}_1^* \rangle\right]}{6}; \tag{2.10}$$

$$\omega_2 = \frac{\operatorname{Im}\left[3\langle \mathbf{B}(\mathbf{U}_1, \mathbf{U}_2), \mathbf{z}_1^* \rangle + \langle \mathbf{C}(\mathbf{U}_1, \mathbf{U}_1, \mathbf{U}_1), \mathbf{z}_1^* \rangle\right]}{3}. \tag{2.11}$$

The solution of the bifurcation problem (1.6), (1.7), and (1.10) takes the form

$$\mu = 0.5\mu_2\varepsilon^2, \quad \omega = \omega_0 + 0.5\omega_2\varepsilon^2, \quad \mathbf{U} = \mathbf{U}_1\varepsilon + 0.5\mathbf{U}_2\varepsilon^2. \tag{2.12}$$

According to [4], the periodic-in-time solution of Eq. (1.10) is stable at the point $\mathbf{U} = 0$ and $\mu = 0$ if $(\partial\mu(\varepsilon)/\partial\varepsilon)\partial\operatorname{Re}\sigma_1/\partial\mu > 0$ and unstable if $(\partial\mu(\varepsilon)/\partial\varepsilon)\partial\operatorname{Re}\sigma_1/\partial\mu < 0$. Using the normalization $\varepsilon = 1$, we conclude that the solution of Eq. (1.10) is stable if $\mu_2 > 0$ and unstable if $\mu_2 < 0$.

The operator $\mathbf{B}(\mathbf{U}, \mathbf{U})$ is a second-order infinitesimal and, in agreement with the statement of [7], Eq. (1.10) has small nonzero solutions in the vicinity of the point $\mu = 0$ for $\mu < 0$ or for $\mu > 0$. Since the operators $\mathbf{A}(\mathbf{U})$, $\mathbf{B}(\mathbf{U}, \mathbf{U})$, and $\mathbf{C}(\mathbf{U}, \mathbf{U}, \mathbf{U})$ are smooth, the solution $\mu \neq 0$ is unique [7]. The stability bound of this solution is defined by the condition

$$\mu - 0.5\mu_2 = 0, \tag{2.13}$$

which is obtained from (2.12) at $\varepsilon = 1$. The solution of the problem (1.6), (1.7), and (1.10) is stable if $\mu - 0.5\mu_2 < 0$ and unstable if $\mu - 0.5\mu_2 > 0$.

Going back to Eq. (1.5) with $\varphi(0,0) = \text{const} \neq 0$, we note that since $\langle \mathbf{\Phi}(0,0), \mathbf{z}_1^* \rangle = 0$, the defect $\mathbf{\Phi}(0,0)$ does not affect the periodic solutions $\mathbf{U}(s) = \mathbf{U}(s + 2n\pi)$ of this equation, and, consequently, (2.13) defines the stability bound of the solutions of the problem (1.5)–(1.7).

As an example, we shall consider the thermal stability of a polytropic chemical reactor for the following initial data: $\beta = 0.2$, $c_0 = 1$, $k_1 = 1$, $k_2 = 0$, $\alpha = 0.6$, $\alpha_1 = 0.1$, and $w = 0.2$. The condition $\mu = \varphi_{1,0} - a = 0$ gives $a = 1$ and $\lambda_1 = 0.374$. In a linear approximation, this permits finding the critical reactor length $l = 3.502$ [by the equation $\tan(\lambda_1 l) - 2\lambda_1 l w^{-1} = 0$], the parameters $\eta = 0.750$, $\Delta_{13} = -0.775$, $\Delta_{21} = 0$, $\Delta_{22} = -1.080$, and $\Delta_{23} = -0.465$ and the vectors

$$z_1 = \|1 \quad -0.75 + 0.194i\|^t \sin(\lambda_1 x)\exp(is), \quad \mathbf{z}_1^* = \|0.353 + 1.365i \quad 1.820i\|^t \sin(\lambda_1 x)\exp(is).$$

As a result of calculation of the scalar products $\langle \mathbf{B}(\mathbf{U}_1, \mathbf{U}_2), \mathbf{z}_1^* \rangle$ and $\langle \mathbf{C}(\mathbf{U}_1, \mathbf{U}_1, \mathbf{U}_1), \mathbf{z}_1^* \rangle$, we find $\operatorname{Re}\langle \mathbf{B}(\mathbf{U}_1, \mathbf{U}_2), \mathbf{z}_1^* \rangle = 0.0137$, $\operatorname{Im}\langle \mathbf{B}(\mathbf{U}_1, \mathbf{U}_2), \mathbf{z}_1^* \rangle = -0.0387$, $\operatorname{Re}\langle \mathbf{C}(\mathbf{U}_1, \mathbf{U}_1, \mathbf{U}_1), \mathbf{z}_1^* \rangle = -0.113$, and $\operatorname{Im}\langle \mathbf{C}(\mathbf{U}_1, \mathbf{U}_1, \mathbf{U}_1), \mathbf{z}_1^* \rangle = 0.104$.

Substitution of the results obtained into (2.10) and (2.11) leads to $\mu_2 = 0.012$ and $\omega_2 = 0.004$, and the solution of the nonlinear problem has the form

$$\mathbf{U} = \mathbf{U}_1\varepsilon + 0.5\mathbf{U}_2\varepsilon^2, \quad \mu = 0.006\varepsilon^2, \quad \omega = 0.194 + 0.002\varepsilon^2. \tag{2.14}$$

Since $\mu_2 > 0$, the bifurcation solution (2.14) of the problem (1.5)–(1.7) is supercritical; it is stable if $\mu < 0.006$. The stability bound, which is determined from (2.14) in the region of small μ for $\varepsilon = 1$, gives the reactor length $l = 3.531$, all other things being equal.

REFERENCES

1. T. A. Bodnar, "Stability of an adiabatic flow-type chemical reactor," *Zh. Prikl. Mekh. Tekh. Fiz.*, No. 3, 91–97 (1991).
2. Ya. B. Zel'dovich, G. I. Barenblatt, V. B. Librovich, et al., *Mathematical Theory of Combustion and Explosion* [in Russian], Nauka, Moscow (1980).
3. T. A. Bodnar, "Thermal stability of a tangent fluid flow in a ring channel," *Zh. Prikl. Mekh. Tekh. Fiz.*, No. 4, 127–133 (1991).
4. J. Joss and D. Joseph, *Elementary Stability and Bifurcation Theory*, New York (1980).
5. B. Hassard, N. Kazarinov, and I. Van, *Theory and Applications of Cycle Birth Bifurcation* [Russian translation], Mir, Moscow (1985).
6. V. V. Kafarov, *Cybernetic Methods in Chemistry and Chemical Technology* [in Russian], Khimiya, Moscow (1976).
7. S. G. Krein (ed.), *Functional Analysis* [in Russian], Nauka, Moscow (1972).