

STABILITY OF A REACTOR COMBINED WITH AN EXTERNAL HEAT EXCHANGER

Yu. I. Kharkats, L. M. Pis'men,
and V. I. Mukosei

UDC 66.021.21

The stability of the stationary regimes of adiabatic reactors operated in such a way that the entering mixture is previously heated by the product flow from the reactor was discussed in several papers [1-3], but none of these papers gave a rigorous solution. The present paper deals with the asymptotic stability of a reactor combined with an external counterflow heat exchanger (Fig. 1). The process considered is assumed to be homogeneous and to involve an arbitrary number of parallel chemical reactions. Ideal prop flow is assumed both for the reactor and for the heat exchanger.

The process in the reactor is described by the set of equations

$$\frac{\partial C_i}{\partial t'} + w \frac{\partial C_i}{\partial x'} = r_i(C_1, \dots, C_k, T), \quad i = 1, 2, \dots, k; \quad (1)$$

$$\frac{\partial T}{\partial t'} + w \frac{\partial T}{\partial x'} = \sum_{i=1}^k h_i r_i(C_1, \dots, C_k, T), \quad (2)$$

where C_i denotes the concentrations of the key substances; T the temperature; t' the time; x' the distance from the reactor inlet; w the linear flow rate; r_i the formation rate of the i -th key substance per unit reactor volume; h_i the reduced thermochemical constant of the i -th key substance.

The process in the heat exchanger is described by the equations

$$\frac{\partial T_1}{\partial t'} + w_1 \frac{\partial T_1}{\partial x''} = \frac{k_T}{\gamma} (T_2 - T_1); \quad (3)$$

$$\frac{\partial T_2}{\partial t'} - w_2 \frac{\partial T_2}{\partial x''} = \frac{k_T}{\gamma} (T_1 - T_2), \quad (4)$$

where T_1 and T_2 denote the temperatures of the hot and cold flows, respectively; k_T the effective coefficient of heat transfer (per unit volume); γ the heat capacity per unit volume of the mixture; w_1 and w_2 the linear velocities of the two flows. Since the conditions for heat exchange are best if $w_1 = w_2$, we shall further consider this case only.

It is convenient to transform Eqs. (1)-(4) into relationships between dimensionless variables

$$\partial u / \partial t + \partial u / \partial x = r(u); \quad (5)$$

$$\partial \tau_1 / \partial t + \partial \tau_1 / \partial x_1 = \alpha(\tau_2 - \tau_1); \quad (6)$$

$$\partial \tau_2 / \partial t - \partial \tau_2 / \partial x_1 = -\alpha(\tau_2 - \tau_1). \quad (7)$$

Here u denotes a $(k+1)$ -dimensional vector the components of which are the k dimensionless concentrations of the key substances u_i ($i = 1, 2, \dots, k$) and the dimensionless temperature u_{k+1} ; r a nonlinear vector function of the vector u ; $t = w_1 t' / l_1$ the dimensionless time; $x = w_1 x' / w l_1$; $x_1 = x'' / l_1$ the dimensionless distance in the heat exchanger; l_1 the length of the heat exchanger; $\alpha = k_T l_1 / \gamma w$.

The asymptotic stability of the reactor is analyzed by studying how small deviations of the variables from the stationary values $u^0(x)$, $\tau_1^0(x_1)$, $\tau_2^0(x_1)$ vary in the course of time. To that end the system (5)-(7) is linearized for solutions close to the stationary regime. We shall search for the following type of partial solutions of the linearized equations

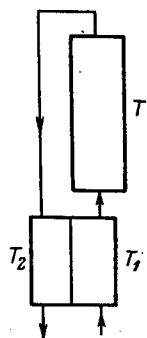


Fig. 1. Flow scheme of a reactor combined with an external heat exchanger.

$$u(x, t) - u^0(x) = e^{\lambda t} v(x), \quad \tau_1(x_1, t) - \tau_1^0(x_1) = e^{\lambda t} \theta_1(x_1),$$

$$\tau_2(x_1, t) - \tau_2^0(x_1) = e^{\lambda t} \theta_2(x_1). \quad (8)$$

The set of equations for the functions $v(x)$, $\theta_1(x_1)$, $\theta_2(x_1)$ then reads

$$dv/dx = A(x)v - \lambda v; \quad (9)$$

$$d\theta_1/dx_1 = \alpha(\theta_2 - \theta_1) - \lambda\theta_1; \quad (10)$$

$$d\theta_2/dx_1 = \alpha(\theta_2 - \theta_1) + \lambda\theta_2, \quad (11)$$

where $A(x)$ denotes the Jacobian matrix of the vector function $r(u)$ with the elements $A_{ij} = (\partial r_i / \partial u_j)_{u=u^0(x)}$. The relationship between the temperature deviations at the inlets and exits of the reactor and the heat exchanger are given by the formulas

$$\theta_1(1) = v_{k+1}(0), \quad \theta_2(1) = v_{k+1}(\beta_1), \quad (12)$$

where $\beta_1 = w_1 l / w l_1$, l the reactor length. The stationary regime is asymptotically stable only if the set of Eqs. (9)-(11) with the boundary conditions (12) and $\theta_1(0) = 0$, $v_i(0) = 0$ ($i = 1, 2, \dots, k$) has a non-trivial solution with $\text{Re } \lambda < 0$.

Let the matrix $V(x)$ be the solution of the equation

$$dV/dx = A(x)V(x) \quad (13)$$

with the initial condition $V(0) = I$ (I is the unit matrix of order $k+1$). Solution of Eq. (9) then yields:

$$v(\beta_1) = V(\beta_1)e^{-\lambda\beta_1}v(0). \quad (14)$$

Substitution of this solution transforms boundary condition (12) into

$$\theta_2(1) = \gamma e^{-\lambda\beta_1} \theta_1(1), \quad (15)$$

where $\gamma = V_{k+1, k+1}(\beta_1)$. If the time lag in the tubular pipes connecting the reactor with the heat exchanger must be taken into account, then, parameter β_1 in the exponent must be replaced by $\beta = \beta_1 + w_1 l_2 / w_2 l_1$, where l_2 denotes the total length of the connecting tubes and w_2 the linear flow rate in these tubes.

Solving the set of Eqs. (10), (11) with the boundary conditions (15) and $\theta_1(0) = 0$, we get the following transcendental equation for λ :

$$\lambda + \alpha + \sqrt{\lambda^2 + 2\lambda\alpha} \coth \sqrt{\lambda^2 + 2\lambda\alpha} = \alpha\gamma \exp(-\beta\lambda). \quad (16)$$

It has to be determined at what values of the parameters α , β , γ all roots of this equation lie on the left of the imaginary axis in the complex plane.

We shall first consider the real roots of Eq. (16). It is easily proved that the plot for the left-hand side of Eq. (16) is a curve which may show some oscillations at $-2\alpha < \lambda < 0$ (the number of oscillations depends on the value of α), and rises monotonically at positive λ , passing at $\lambda = 0$ through the point with the ordinate $1 + \alpha$ on the vertical axis. This curve intersects the exponential curve in several points (in one point, if there are no oscillations) which yield the real roots of Eq. (16) (see Fig. 2). The position of the root on the extreme right depends on the value of parameter γ : at $\gamma > (1 + \alpha)/\alpha$ all real roots of Eq. (16) are negative.

We shall now prove that all complex roots of Eq. (16) lie in the left semiplane, whereas the real root is shifted into the right semiplane when parameter γ increases. To do so, it suffices to prove that at $\gamma = (1 + \alpha)/\alpha$ the right and left-hand sides of Eq. (6) map the right-hand semiplane of the complex λ plane into nonintersecting regions at all values of parameters α and β . The right-hand side of Eq. (16) maps the right-hand λ semiplane into the interior region of the circle with radius $1 + \alpha$. Application of the left-hand side of Eq. (16) maps the right-hand semiplane into the region which is bounded on the left by the curve generated by mapping the imaginary axis of the λ plane. Let $\lambda = iy$, $y > 0$ (at $y < 0$ the curve is symmetric with respect to the real axis). Separating the real and imaginary parts, we then find the parametric equations of the curve sought

$$u = \alpha + (a \operatorname{sh} 2a + b \sin 2b) / 2(\operatorname{sh}^2 a + \sin^2 b); \quad (17)$$

$$v = y + (b \operatorname{sh} 2a - a \sin 2b) / 2(\operatorname{sh}^2 a + \sin^2 b), \quad (18)$$

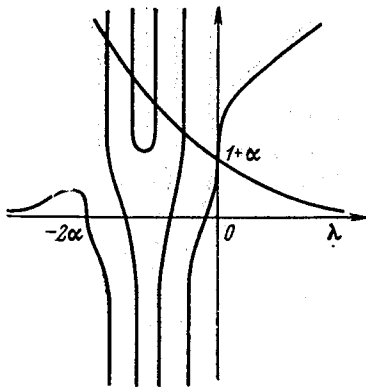


Fig. 2. Position of the real roots of Eq. (16).

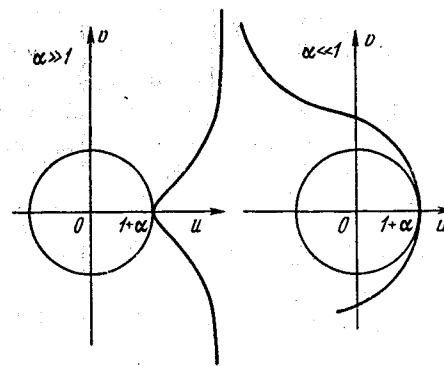


Fig. 3. Position of the circle with radius $1 + \alpha$ with respect to the curve at $\alpha \gg 1$ and $\alpha \ll 1$.

where

$$a = [(y^4/4 + \alpha^2 y^2)^{1/2} - y^2/2]^{1/2}, \quad b = [(y^4/4 + \alpha^2 y^2)^{1/2} + y^2/2]^{1/2}. \quad (19)$$

We shall consider the positions of the curve with respect to the circle with radius $1 + \alpha$ in the limiting cases $\alpha \gg 1$ and $\alpha \ll 1$. If $\alpha \gg 1$ and y are so small that $a \approx b \sqrt{\alpha y} \ll 1$, we find from (17), (18)

$$u = \alpha + 1 + \frac{4}{45} \alpha^2 y^2; \quad (20)$$

$$v = y + \frac{2}{3} \alpha y. \quad (21)$$

We see that the curve touches the circle at $y = 0$ and moves away at rising y . If y is further increased so that $y \sim \alpha$, we find

$$u = \alpha + a + b \sin 2b/a \operatorname{sh} 2a - \sin^2 b / \operatorname{sh}^2 a; \quad (22)$$

$$v = y + b - a \sin 2b/b \operatorname{sh} 2a - \sin^2 b / \operatorname{sh}^2 a. \quad (23)$$

The curve in this range of y values is determined by the two first terms in (22) and (23); the other terms are corrections which produce loops of very small amplitude in the curve.

Since at $y > 1 + \alpha$ the curve certainly cannot intersect the circle with radius $1 + \alpha$, we are not further interested in the behavior of the curve at $\alpha \gg 1$ (see Fig. 3). Considering the curve at $\alpha \ll 1$, we note that at $y \sim \alpha$

$$u = 1 + \alpha + (a^2 - b^2)/3, \quad (24)$$

$$v = y + \frac{2}{3} ab^3 / (a^2 + b^2). \quad (25)$$

Starting at very low y values, we may take that $a \approx \alpha$, $b \approx y$ and get the parametric equations of the curve:

$$u = \alpha + (\alpha \operatorname{sh} 2\alpha + y \sin 2y) / 2(\operatorname{sh}^2 \alpha + \sin^2 y); \quad (26)$$

$$v = y + (y \operatorname{sh} 2\alpha - \alpha \sin 2y) / 2(\operatorname{sh}^2 \alpha + \sin^2 y). \quad (27)$$

From Eqs. (24)-(27) it is evident that the curve at $\alpha \ll 1$ touches the circle at $y = 0$, and then, bending around the circle, passes through the point $(\pi/4, \pi/4)$ and intersects the imaginary axis first at $y \approx \pi/2$. The further path of the curve is shown in Fig. 3.

Consequently, neither it $\alpha \ll 1$ does the curve intersect the circle, but solely touches it at $y = 0$. At all other α values the position of the curve with respect to the circle is intermediate between the two extreme cases considered, and it may be stated that the appearance of unstable regimes is related to transfer of the real root to the right semiplane.

The critical value of parameter γ , which equals $(1 + \alpha)/\alpha$, corresponds to a stationary regime for which there exist two nearly identical regimes for slightly different values of the parameters (branching point of the solutions) for the stationary linearized equations derived from (5)-(7) have a nontrivial solution for these parameter values. Consequently, the condition for reactor stability reads

$$\gamma < (\alpha + 1) / \alpha, \quad (28)$$

and transition from a stable to an unstable regime takes place only in the branching points of the solutions of the stationary equations. To check condition (28), it suffices to calculate parameter γ , which, as is easily seen from Eq. (13), equals the parametric sensitivity of the temperature near the reactor exit to the inlet temperature. In particular, simple calculations of a zero-order reaction with the rate constant $k(t)$ yield the equation

$$\gamma = k[T(\beta_1)] / k[T(0)], \quad (29)$$

i.e., in this case, parameter γ equals the ratio of the rate constants at the reactor exit and inlet.

LITERATURE CITED

1. C. van Heerden, *Ind. and Eng. Chem.*, **45**, 1232 (1953).
2. M. G. Slin'ko and A. L. Muller, *Kinetika i Kataliz*, **2**, 467 (1961).
3. G. K. Orcatt and D.E. Lamb, *First International IFAK Congress on Automatic Control [in Russian]*, Vol. 6, Izd. AN SSSR (1960).