NONISOTHERMAL MULTICOMPONENT SORPTION DYNAMICS IN POROUS MEDIA FOR CONSIDERABLY DIFFERING MASS-TRANSFER COEFFICIENTS

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Solutions of the equations of multicomponent nonisothermal sorption dynamics are analyzed. It is shown that inversion occurs when the mass-transfer coefficient of the weakly sorbed component is very low.

Nonisothermal multicomponent sorption dynamics in porous media is described by a system consisting of material-balance equations for each component of the mixture, thermal sorption equations [Eq. (1)], model kinetic equations for each mixture component [Eq. (2)], heat-balance equations, model kinetic equations of heat transfer [Eq. (3)], and initial and boundary conditions [Eq. (4)]:

$$\alpha_m \frac{\partial q_m}{\partial t} + \frac{\partial c_m}{\partial z} = 0,\ m = 1,2,\ \ldots\ n,\ q_m = f_m(c_1',\ \ldots,\ c_n',\ \overset{*}{T}), \tag{1}$$

$$\alpha_m \frac{\partial q_m}{\partial t} = \Omega_m(x_m)\,[f_m(c_1,\ \ldots,\ c_n,\ \overset{*}{T}) - q_m],\ x_m = q_m/f_m(c_1,\ \ldots,\ c_n,\ \overset{*}{T}), \tag{2}$$

$$\Omega_m(x_m) = g_m(x_m)\{\alpha_{0m} + \gamma_m^0 + \gamma_m[\omega_m(x_m)]^{-1}\}^{-1},$$

$$\frac{\partial \overset{*}{T}}{\partial t} = m_3(T - \overset{*}{T}) + \sum_{m=1}^{n} Q_m \frac{\partial q_m}{\partial t},\quad \frac{\partial T}{\partial z} = m_1(T - \overset{*}{T}) - m_2 T, \tag{3}$$

$$c_m(z,\ 0) = b_m,\ T(z,\ 0) = \overset{*}{T}(z,\ 0) = T(0,\ t) = 0, \tag{4}$$

$$c_m(0,\ t) = F_m(t),\ q_m(0,\ t) = F_m^0(t),\quad \overset{*}{T}(0,\ t) = H(t).$$

To ensure continuity of the solutions, the functions $F_m^0(t)$ and $H(t)$ must be determined from the equations

$$\alpha_m \frac{dF_m^0}{dt} = \Omega_m(x_m^0)\,[f_m(F_1,\ \ldots,\ F_n,\ H) - F_m^0],$$
$$F_m^0(0) = f_m(b_1,\ \ldots,\ b_n,\ 0), \tag{5}$$
$$\frac{dH}{dt} = -m_3 H + \sum_{m=1}^{n} Q_m \frac{dF_m^0}{dt},\ H(0) = 0,\ x_m^0 = F_m^0/f_m(F_1,\ \ldots,\ F_n,\ H).$$

The method of determining ω_m was given in [1, 2], together with analytical expressions for ω_{0m} for sorption and ω_m^0 for desorption. The model kinetic equations given in Eq. (2) are valid for porous media consisting of porous grains, the effective pore size of which is comparable with the molecular dimensions of the mixture being sorbed. If the effective pore size is significantly larger than the molecular dimensions of the mixture being sorbed, it is necessary to use the kinetic equations given as Eq. (1.1) in [2]. In order to integrate Eqs. (1)-(5) for arbitrary initial and boundary conditions and arbitrary form of the function f_m, it is necessary to use a difference scheme [3]. An implicit monotonic iterative conservative difference scheme of accuracy $O(h^2 + \tau)$ for Eqs. (1)-(3) takes the form

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$$c_{m,i+1}^{(s+1)\,j+1} = c_{m,i}^{(s+1)\,j+1} - h\Omega_m [q_{m,i}^{(s+1)\,j+1}/f_m (c_{1,i+1/2}^{(s)\,j+1}, \ \ldots, \ c_{n,i+1/2}^{(s)\,j+1}, \ \overset{*}{T}{}_i^{(s+1)\,j+1})] \times$$

$$\times [f_m (c_{1,i+1/2}^{(s)\,j+1}, \ \ldots, \ c_{n,i+1/2}^{(s)\,j+1}, \ \overset{*}{T}{}_i^{(s+1)\,j+1}) - q_{m,i}^{(s+1)\,j+1} +$$

$$+ (c_{m,i+1/2}^{(s+1)\,j+1} - c_{m,i+1/2}^{(s)\,j+1}) \ \frac{\partial f_m}{\partial c_m} \ (c_{1,i+1/2}^{(s)\,j+1}, \ \ldots, \ c_{n,i+1/2}^{(s)\,j+1}, \ \overset{*}{T}{}_i^{(s+1)\,j+1})],$$

$$q_{m,i}^{(s+1)\,j+1} = q_{m,i}^{j} + \frac{\tau}{\alpha_m} \ \Omega_m [q_{m,i}^{(s)\,j+1}/f_m (c_{1,i+1/2}^{(s)\,j+1}, \ldots, \ c_{n,i+1/2}^{(s)\,j+1}, \ \overset{*}{T}{}_i^{(s)\,j+1})] \times$$

$$\times [f_m (c_{1,i+1/2}^{(s)\,j+1}, \ \ldots, \ c_{n,i+1/2}, \ \overset{*}{T}{}_i^{(s)\,j+1}) - q_{m,i}^{(s)\,j+1}], \tag{6}$$

$$T_{i+1}^{(s+1)\,j+1} = T_i^{(s)\,j+1} - h (m_1 + m_2) \ T_{i+1/2}^{(s)\,j+1} + m_1 h \overset{*}{T}{}_i^{(s+1)\,j+1},$$

$$\overset{*}{T}{}_i^{(s+1)\,j+1} = \overset{*}{T}{}_i^{j} + \tau m_3 (T_{i+1/2}^{(s)\,j+1} - \overset{*}{T}{}_i^{(s)\,j+1}) +$$

$$+ \tau \sum Q_m/\alpha_m \Omega_m [q_{m,i}^{(s)\,j+1}/f_m (c_{1,i+1/2}^{(s)\,j+1}, \ \ldots, \ c_{n,i+1/2}^{(s)\,j+1}, \ \overset{*}{T}{}_i^{(s)\,j+1})] \times$$

$$\times [f_m (c_{1,i+1/2}^{(s)\,j+1}, \ \ldots, \ c_{n,i+1/2}^{(s)\,j+1}, \ \overset{*}{T}{}_i^{(s)\,j+1}) - q_{m,i}^{(s)\,j+1}].$$

The advantage of Eq. (6) is that continuous calculations for it converge to a class of discontinuous coefficients. Using the scheme in Eq. (6), which is linearized for error, and estimating the norm of the corresponding matrices, we can find necessary and sufficient conditions for the convergence of the iterative process, which will be satisfied if

$$\tau_m \leqslant \Big| 1 + 1/2\, hF_m^0 \sum_{m=1}^{n} H_{mp} \Big| \Big\{ |F_m/\alpha_m + F_m^0 H_m \sum_{s=1}^{n} Q_s/\alpha_s +$$

$$+ F_m F_m^0 h/\alpha_m \sum_{p=1}^{n} H_{mp} + hF_m^0 H_m \sum_{s=1}^{n} F_s^0 \, Q_s/\alpha_s \sum_{p=1}^{n} H_{sp} \Big| +$$

$$+ h \Big| H_m F_m^0 (F_m^0/\alpha_m - m_3/2 + \sum_{s=1}^{n} Q_s F_s^0 \, H_s/\alpha_s) \Big| + 1/2\, m_3 h \, |H_m F_m^0| \Big\}^{-1},$$

$$F_m^0 = \Omega_m \frac{\partial \Omega_m}{\partial x_m} \ (f_m - q_m)\, x_m/f_m, \ \ H_m = \partial f_m/\partial \overset{*}{T}, \tag{7}$$

$$\tau_1 \leqslant \Big\{ m_3 + \Big| 2 \sum_{m=1}^{n} Q_m H_m F_m^0/\alpha_m - m_3 \Big| + \sum_{p=1}^{n} 2\, |F_m^0 H_{mp}|\, Q_m/\alpha_m \ + \sum_{m=1}^{n} Q_m (|1 - hF_m^0 H_{mp}| + |1 + hF_m^0 H_{mp}|)/(\alpha_m h) \Big\}^{-1},$$

$$F_m = \Omega_m - \frac{\partial \Omega_m}{\partial x_m} \ (f_m - q_m)/f_m, \ \ \tau = \min\{\tau_1, \ \tau_m\}, \ \ H_{mp} = \partial f_m/\partial c_p.$$

When Eq. (7) is satisfied, the necessary and sufficient condition for the absolute stability and convergence of the difference scheme in Eq. (6) is fulfilled. The coefficients in Eqs. (1)-(4) differ: for sorption, $f_m \to f_m$, $\omega_m \to \omega_{0m}$, and $\gamma_m \to \gamma_m$; for desorption, $f_m \to f_m^0$, $\omega_m \to \omega_m^0$, and $\gamma_m \to \gamma_m^*$. In order to determine the conditions for which sorption or desorption occurs, it is necessary to use the inequalities

$$q_{m,0}^{(s)\,j+1} \geqslant q_{m,0}^{j}, \ \ q_{m,0}^{(s)\,j+1} < q_{m,0}^{j}, \tag{8}$$

$$f_{m,i+1/2}^{(s)\,j+1} \geqslant q_{m,i+1/2}^{(s)\,j+1}, \ \ f_{m,i+1/2}^{(s)\,j+1} > q_{m,i+1/2}^{(s)\,j+1}. \tag{9}$$

When the first inequality in Eq. (8) is satisfied, $f_m \to f_m$ in Eq. (9); when the second is satisfied, $f_m \to f_m^0$ in Eq. (9). When the first inequality in Eq. (9) is satisfied, sorption occurs, and when the second inequality is satisfied, desorption occurs. When the first inequality of Eq. (10) is satisfied, heating of the porous medium occurs, and in Eq. (3) it is necessary to make the substitutions $m_1 \to m_1$, $m_3 \to m_3$:

$$\overset{*}{T}{}_i^{(s)\,j+1} \geqslant T_{i+1/2}^{(s)\,j+1}, \ \ \overset{*}{T}{}_i^{(s)\,j+1} < T_{i+1/2}^{(s)\,j+1}. \tag{10}$$

When the second inequality of Eq. (10) is satisfied, the porous medium is cooled by a gas–liquid flow, and in Eq. (3) it is necessary to make the substitutions $m_1 \to m_1^0$, $m_3 \to m_3^0$. For numerical integration, Eqs. (9) and (10) must be verified at each grid point i. As an example, using the difference scheme in Eq. (6) for the Langmuir thermal functions

$$f_m = p_m c_m s_m \Big[1 + \sum_{m=1}^{n} p_m c_m s_m \Big]^{-1}, \ \ s_m = \exp[-Q_{*m}\overset{*}{T}/(1 + \overset{*}{T})], \ \ \varphi_m = f_m^{-1} \tag{11}$$

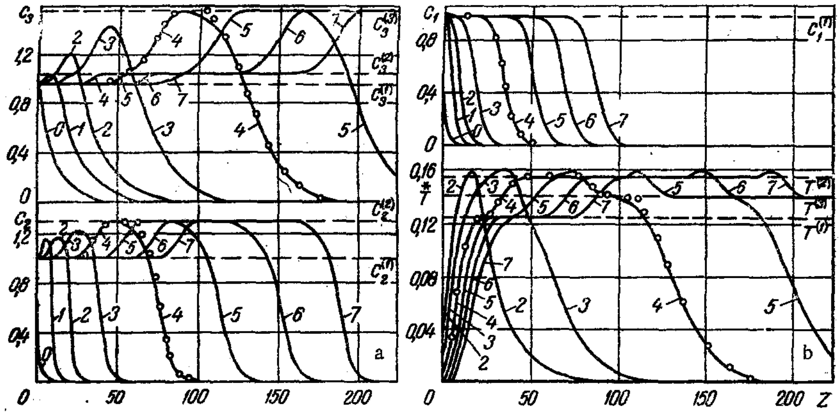

Fig. 1. Frontal isothermal dynamic curves for three-component mixture: 0) t = 0; 1) 5; 2) 10; 3) 20; 4) 40; 5) 60; 6) 80; 7) 100. The points show invariant solutions of Eq. (20).

frontal dynamic curves were calculated on a BESM-6 computer for a three-component mixture with the following parameters:

$$\Omega_1 = \Omega_2 = 1,\ \Omega_3 = 0.1,\ Q_1 = 0.1,\ Q_2 = 0.2,\ Q_3 = 0.3,\ m_1 = 1,$$
$$m_2 = 0,\ m_3 = 0.2,\ \alpha_1 = 2.5,\ \alpha_2 = 1.5,\ \alpha_3 = 1,\ n = 3,\ p_1 = 4,$$
$$p_2 = 2,\ p_3 = 1,\ Q_{*m} = 5,\ b_m = 0,\ F_m(t) = 1.$$

The results of the integration are shown in Fig. 1a, b. From an analysis of the nonisothermal frontal dynamic curves, it is evident that in porous media four stationary concentration and temperature fronts are formed ($W_1 = 0.184$, $W_2 = 0.86$, $W_3 = 1.85$, $W_4 = 3.42$; $c_1^{(0)} = 1$, $c_1^{(1)} = 0.9784$, $c_1^{(2)} = 0$, $c_2^{(0)} = 1$, $c_2^{(1)} = 0.9945$, $c_2^{(2)} = 1.29$, $c_2^{(3)} = 0$, $c_3^{(0)} = 1$, $c_3^{(1)} = 0.9981$, $c_3^{(2)} = 1.06$, $c_3^{(3)} = 1.56$, $c_3^{(4)} = 0$, $T^{(0)} = 0$, $T^{(1)} = 0.124$, $T^{(2)} = 0.154$, $T^{(3)} = 0.141$, $T^{(4)} = 0$). For Langmuir thermal functions with comparable values of the mass-transfer coefficient, there is no inversion. If one weakly sorbed mixture component has a mass-transfer coefficient significantly lower than the others, inversion occurs (at first, the strongly sorbed component propagates more rapidly along the porous medium and then, after a certain lapse of time, it "overtakes" the weakly sorbed component). In the example shown in Fig. 1, for $0 \le t \le t_* = 7.5$, the second component propagates more rapidly along the porous medium at high temperatures and, for $t > t_*$, it overtakes the weakly sorbed third component. The value of t_* increases as the difference between the coefficients of the second and third mixture components increases. Equations (1)-(3) permit the existence of invariant solutions of traveling-wave type (stationary fronts) [4] for $m_2 = 0$. In the traveling-wave mode, as $m_1, m_3 \to \infty$, this system can be written, after rearrangement, in the form

$$\frac{dc_m}{dy} = \Omega_m(x_m^*)\,[q_m^{(p)} - f_m(c_1, \ldots, c_n, G_p(c)) + (c_m - c_m^{(p)})(\alpha_m W_p)^{-1}] = \Omega_m(x_m^*)\,R_m^{(p)}(c), \tag{12}$$

$$q_m = q_m^{(p)} + (c_m - c_m^{(p)})(\alpha_m W_p)^{-1},\quad y = z - W_p t, \tag{13}$$
$$x_m^* = q_m(c_m)/f_m(c, G_p(c)),$$

$$W_p = (c_m^{(p+1)} - c_m^{(p)})\,[(q_m^{(p+1)} - q_m^{(p)})\,\alpha_m]^{-1},\quad T^{(p+1)} = G_p(c^{(p+1)}), \tag{14}$$

$$T = T^{(p)} + \sum_{m=1}^{n} Q_m (c_m - c_m^{(p)})\,[\alpha_m (W_p - a)]^{-1} = G_p(c),\quad a = m_3/m_1, \tag{15}$$

$$R_m^{(p)}(c^{(p)}) = R_m^{(p)}(c^{(p+1)}) = 0, \tag{16}$$

where $q_m^{(p)}$, $c_m^{(p)}$, $T^{(p)}$, $q_m^{(p+1)}$, $c_m^{(p+1)}$, $T^{(p+1)}$ are values of the equilibrium concentration and temperature at the left and right, respectively, along the porous medium for a traveling p-wave; W_p is the velocity of propagation of the traveling p-wave. If, assuming Eq. (16) and an arbitrary form of the function f_m, the solutions $c_m(y)$ of Eq. (12) are to be monotonic, the functions $R_m^p(c)$ should not change sign for $c_m^{(p)} \le c_m \le c_m^{(p+1)}$. Multiplying Eq. (12) successively by $c_m - c_m^{(p)}$ and $c_m - c_m^{(p+1)}$ and rearranging, we obtain

$$\frac{f_m(c_1, \ldots, c_n, G_p(c)) - q_m^{(p)}}{c_m - c_m^{(p)}} > \frac{1}{\alpha_m W_p} \geqslant \frac{f_m(c_1, \ldots, c_n, G_p(c)) - q_m^{(p+1)}}{c_m - c_m^{(p+1)}}. \tag{17}$$

For $c_m^{(p+1)} < c_m^{(p)}$, the sign of the inequalities must be reversed. To determine the monotonic concentra-

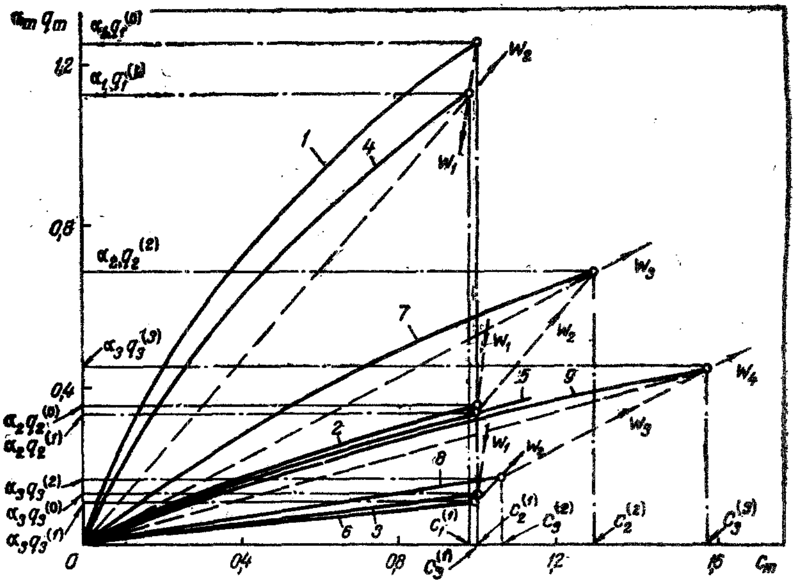

Fig. 2. Thermal functions: 1) $\alpha_1 q_1 (c_1, c_2^{(0)}, c_3^{(0)}, 0)$; 2) $\alpha_2 q_2 (c_1^{(0)}, c_2, c_3^{(0)}, 0)$; 3) $\alpha_3 q_3 (c_1^{(0)}, c_2^{(0)}, c_3, 0)$; 4) $\alpha_1 q_1 (c_1, c_2^{(1)}, c_3^{(1)}, T^{(1)})$; 5) $\alpha_2 q_2 (c_1^{(1)}, c_2, c_3^{(1)}, T^{(1)})$; 6) $\alpha_3 q_3 (c_1^{(1)}, c_2^{(1)}, c_3, T^{(1)})$; 7) $\alpha_2 q_2 (c_1^{(2)}, c_2, 0, T^{(2)})$; 8) $\alpha_3 q_3 (0, c_2^{(2)}, c_3, T^{(2)})$; 9) $\alpha_3 q_3 (0, 0, c_3, T^{(3)})$.

tion distribution in the wave traveling with velocity W_p, we divide the system in Eq. (12) by its s-th equation, to obtain

$$dc_m/dc_s = \Omega_m (x_m^*) R_m^{(p)} (c) [\Omega_s (x_s^*) R_s^{(p)} (c)]^{-1}, \quad m \neq s. \tag{18}$$

Integrating the system of ordinary equations by Runge's method, and verifying at each successive step of the integration the necessary and sufficient conditions – Eqs. (23) and (17), respectively – for the existence of invariant solutions of traveling-wave type, we find $c_m = P_m(c_s)$. We substitute the solutions $P_m(c_s)$ obtained into the right-hand side of the s-th equation of the system in Eq. (12):

$$dc_s/dy = \Omega_s (c_s) R_s^{(p)} (P_1 (c_s), \ldots, c_s, \ldots, P_n (c_s), G_p (c_s)) = F_s^* (c_s). \tag{19}$$

Hence, we find the solutions of the system in Eq. (12) in the form ($a = c_s^{(p)}$, $b = c_s^{(p+1)}$)

$$c_s = \Phi_s (y - y_0), \; c_m = P_m (\Phi_s (y - y_0)), \; y_0 = \int_a^b \Phi_s^{-1} (c_s)\, dc_s, \; \Phi_s^{-1} = \int [F_s^* (c_s)]^{-1} dc_s. \tag{20}$$

If the kinetic rate of heat and mass transfer Ω_m is large, and $m_1, m_3 \to \infty$, then Eqs. (1)-(3) are transformed to give

$$\frac{\partial v_m}{\partial t} + B_{im} (v) \frac{\partial v_m}{\partial z} = 0, \quad v_m = \begin{pmatrix} q_m \\ T \end{pmatrix}, \tag{21}$$

where B_{im} is a matrix with elements

$$b_{im} = \frac{\partial \varphi_i}{\alpha_i \partial q_m}, \; b_{i(n+1)} = \frac{\partial \varphi_i}{\alpha_i \partial T}, \; b_{(n+1)i} = \sum_{m=1}^{n} \frac{Q_m \partial \varphi_m}{\alpha_m \partial q_i}, \quad b_{(n+1)(n+1)} = a + \sum_{m=1}^{n} \frac{Q_m \partial \varphi_m}{\alpha_m \partial T}.$$

Only three types of invariant solution of Eq. (21) can exist: constant solutions q_m, $T = \text{const}$; discontinuous solutions of traveling-wave type [the monotonic solutions of traveling-wave form in Eq. (20) transform to discontinuous solutions when $\Omega_m \to \infty$]; and self-modeling invariant solutions of spreading-wave type, which are found by solving the system

$$[y\delta_{im} - B_{im} (v)] \frac{dv_m}{dy} = 0, \quad y = z/t. \tag{22}$$

The necessary conditions for the existence of $n+1$ invariant solutions of traveling-wave or spreading-wave type is the existence of $n+1$ different roots λ_i of the matrix B_{im}, where

$$0 < \lambda_1 < \lambda_2 < \ldots < \lambda_n < \lambda_{n+1}. \tag{23}$$

If q_m, $T \neq$ const, solutions of Eq. (22) are found from the system

$$y = \lambda_p(v) = \lambda_p(q, T), \quad (24)$$

$$dv_m/dy = br_m^{(p)}(v), \; b = \sum_{m=1}^{n} (\partial\lambda_p/\partial q_m)\, r_m^{(p)} + (\partial\lambda_p/\partial T)\, r_{n+1}^{(p)}, \quad (25)$$

where $r_m^{(p)}(v)$ is the right eigenvector of matrix B_{im} corresponding to the eigenvalue λ_p. For monotonic decrease (increase), the solutions of Eq. (25) should satisfy the condition

$$br_m^{(p)}(v) < 0 \; (br_m^{(p)}(v) > 0). \quad (26)$$

We divide the system in Eq. (25) by its (n + 1)-th equation, to obtain

$$dq_m/dT = r_m^{(p)}(v)/r_{n+1}^{(p)}(v), \; m \leqslant n. \quad (27)$$

Integrating the system of ordinary equations and verifying at each integration step that Eqs. (23) and (26) are satisfied, we find $q_m = G_m^*(T)$. We substitute the solutions obtained into Eq. (24) and find the self-modeling solutions

$$T = \Psi_p(y), \; q_m = G_m^*(\Psi_p(y)), \; \Psi_p^{-1}(T) = \lambda_p(G_1^*(T), \ldots, G_n^*(T), T). \quad (28)$$

Each invariant solution is determined by one unknown parameter. It is convenient to take $q_p^{(p+1)}$ and $T^{(p+1)}$ as the unknown parameters; for the traveling-wave and spreading-wave modes, these parameters are determined by the method of successive approximation in such a way as to satisfy Eq. (4). For applications, it is of interest to analyze the equations of motion of the mixture [Eqs. (1)-(3)] for the Langmuir functions in Eq. (11). Taking into account the substitutions $Q_m q_m \to q_m$, $Q_m c_m \to c_m$, we write for Eq. (21) the characteristic equation from which we find the eigenvalue λ of the matrix B_{im}:

$$a - \lambda = H(\lambda, q) = \sum_{m=1}^{n} (\lambda - a + \lambda b_m)\, q_m \lambda_m^* \,[(\lambda_m^* - \lambda) V]^{-1}, \quad (29)$$

$$V = 1 - \sum_{m=1}^{n} q_m, \; b_m = -V\partial(\ln s_m)/\partial T > 0, \; \lambda_m^* = (\alpha_m p_m s_m V)^{-1}.$$

We shall show that for

$$0 < a < \lambda_n^*(1 + b_n) \quad (30)$$

there are n + 1 roots λ_p of Eq. (29). We assume that $\lambda_i^*(1 + b_i) < a < \lambda_{i+1}^*(1 + b_{i+1})$. Since the function $H(\lambda, q)$ has a pole at the point λ_m^* $(1 \leq m \leq n)$, decreases monotonically for $\lambda \leq \lambda_i^*$, and rises monotonically for $\lambda \geq \lambda_{i+1}^*$, Eq. (29) has i roots in the region $0 \leq \lambda \leq \lambda_i^*$ and $n - i - 1$ roots in the region $\lambda \geq \lambda_{i+1}^*$. The function $\partial H/\partial\lambda$ increases monotonically in the region $\lambda_i^* \leq \lambda \leq \lambda_{i+1}^*$ and has one zero, and so the function $H(\lambda, q)$ has one minimum in this region. The sufficient condition for $H(\lambda, q)$ to have two different roots $\lambda_i < \lambda_i^0$ in this region is

$$H(\lambda_{1/2}, q) < 1/2\,[H(\lambda_i, q) + H(\lambda_i^0, q)] = a - \lambda_{1/2}, \; \lambda_{1/2} = 1/2\,(\lambda_i + \lambda_i^0). \quad (31)$$

Taking Eq. (29) into account, we transform Eq. (31) to the obvious inequality

$$\sum_{p=1}^{n} q_p \lambda_p^* \,[(\lambda_p^*(1 + b_p) - a]\,(\lambda_i\lambda_i^0 - \lambda_{1/2}^2)\,[V(\lambda_p^* - \lambda_{1/2})(\lambda_p^* - \lambda_i)(\lambda_p^* - \lambda_i^0)]^{-1} < 0. \quad (32)$$

From the foregoing it follows that, when Eq. (30) is satisfied, the Langmuir thermal function permits the existence of n + 1 invariant solutions in the porous medium. If $a > \lambda_n^*(1 + b_n)$, the thermal-wave velocity a is larger than the concentration-wave velocity, and the heat liberated (absorbed) is rapidly carried away along the porous medium. In this case, the sorption dynamics may be assumed to be isothermal. If $a > \lambda_n^*(1 + b_n)$, the function $H(\lambda, q)$ is monotonically decreasing, and Eq. (29) permits the existence of n roots. The right $[r_m^{(p)}, r_{n+1}^{(p)}]$ and left $[l_m^{(p)}, l_{n+1}^{(p)}]$ eigenvectors of matrix B_{im} are

$$r_m^{(p)} = (a/\lambda_p - 1 - b_m)\, q_m \lambda_m^* (\lambda_m^* - \lambda_p)^{-1}, \; r_{n+1}^{(p)} = 1,$$

$$l_m^{(p)} = q_m \lambda_m^* \,[(\lambda_m^* - \lambda_p) V]^{-1}, \; l_{n+1}^{(p)} = (1 - a/\lambda_p)^{-1} \sum^{n} b_m q_m \lambda_m^* \,[(\lambda_m^* - \lambda_p) V]^{-1}.$$

Given the unknown parameter $T^{(1)}$ [the other parameters are known, since $c_p^{(p+1)} = 0$] and using an iterative graphical-analytic method based on linear concentration and temperature dependences – Eqs. (13) and (15), respectively – we can determine the equilibrium values of concentration and temperature in the traveling-wave mode for a mixture of any number of components, without carrying out numerical calculations on a computer. The calculation sequence for the iterative method in the case of a three-component mixture with the parameters of the above example is shown in Fig. 2. The iteration is terminated when the difference between successive iterations is less than the given accuracy of the calculation.

NOTATION

c_m, concentration of m-th mixture component in gas–liquid flow; q_m, concentration of m-th component absorbed by the medium; ω_m, function describing the filling of the porous grain; g_m, function taking into account dependence of diffusion coefficient inside porous grain; γ_m^0, relative critical coefficient taking into account mass transfer on external boundary of porous grain; γ_m, relative critical coefficient taking into account mass transfer inside porous grain; α_{0m}, relative coefficient taking into account mass transfer due to longitudinal effective mixing; m_1, m_3, relative coefficients of heat transfer between gas flow and porous grains; m_2, relative coefficient of heat transfer with external surface of channel composed of porous grains; Q_m, relative thermal effect of sorption (desorption).

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STEADY-STATE TEMPERATURE FIELD OF A WALL WITH CYLINDRICAL COOLING CHANNELS

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The Bubnov–Galerkin method is combined with the structural method worked out by Rvachev to solve the problem of the steady-state temperature field of a wall with cylindrical cooling channels in a two-row arrangement.

We consider a flat wall ($-b \leq y \leq b$, $-\infty < x$, $z < \infty$), in which there are cylindrical cooling channels of radius r, arranged as in Fig. 1a. The wall material has a constant thermal conductivity λ. At the surfaces $y = \pm b$ the wall is heated by the surrounding gas which is at temperature T_1; the heat-transfer coefficient is α_1. This heat is transferred to the massive wall of the cooling liquid with temperature T_2; the heat-transfer coefficient of the surface of a channel containing liquid is α_2. We are to determine the steady-state temperature field of the wall. To do this, we combine the Bubnov–Galerkin method with the structural method worked out by Rvachev [1-3].

Making use of the symmetry of this unknown temperature field, we can reduce the problem to that of solving the Laplace equation in region Ω (Fig. 1a):

$$A\Theta = -\Delta\Theta = -\left(\frac{\partial^2\Theta}{\partial x_1^2} + \frac{\partial^2\Theta}{\partial x_2^2}\right) = 0,\ x = (x_1,\ x_2) \in \Omega \tag{1}$$

with the boundary conditions

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