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NUMERICAL SOLUTION OF AN INVERSE PROBLEM IN NONSTATIONARY MASS TRANSFER IN A MULTICOMPONENT MIXTURE

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Discrepancy-functional minimization is used to show that there is considerable interaction between adsorbed components during transport in a porous material.

A major problem in the theory of heat and mass transfer concerns methods of solving inverse problems, which have been classified in [1-3]; one needs numerical values for the kinetic coefficients to simulate and optimize mass-transfer equipment. To determine these for mixtures, it is necessary to solve for kinetic-parameter matrices [4]. One measures the concentrations averaged over the volumes of the porous particles, which are dependent on run time (kinetic curves) when one examines nonstationary transfer in sorbents and catalysts. An inverse problem in mass transfer for a binary mixture can [5] be handled by determining the elements in the coefficient matrix by using sections of the kinetic curves. Here we consider a method of solving for nonstationary mass transfer for an n-component mixture, which is based on minimizing the discrepancy functional, where it is shown that there is a considerable interaction between the components within the material.

The mass flux densities are put as [6]

$$j = -D\nabla a. \tag{1}$$

We consider the simplest case of boundary conditions of the first kind. The equations for nonstationary mass transfer for an n-component mixture subject to constant values for the elements of matrix D may be written as

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$$\frac{\partial a}{\partial t} = D\left(\frac{\partial^2}{\partial x^2} + \frac{\Gamma}{x}\frac{\partial}{\partial x}\right)a,$$
$$a(x,\ 0) = 0,\quad \left.\frac{\partial a}{\partial x}\right|_{x=0} = 0,\quad a(R,\ t) = a_0. \tag{2}$$

The solution to (2) for the means over the volumes of

$$\bar{a}(t) = \frac{\Gamma+1}{R^{\Gamma+1}}\int_0^R x^\Gamma a(x,\ t)\,dx$$

is

$$\bar{a}(t) = \left[I - \frac{2(1+\Gamma)}{\pi^2}\sum_{m=1}^{\infty}\frac{1}{m^2}\exp(-m^2\pi^2 Dt)\right]a_0. \tag{3}$$

It follows from (3) that the concentration vector $\bar{a}$ is a function of D; solving the inverse problem amounts to determining D from the experimental $\bar{a}_{ex}(t)$. From (3) we get a quadratic function of the discrepancies:

$$f(D) = \sum_{i=1}^{q}\|\bar{a}(t_i) - \bar{a}_{ex}(t_i)\|^2. \tag{4}$$

The elements of D are derived by minimizing f(D); D should have eigenvalues with positive real parts, since otherwise the matrix series in (3) will diverge and the solution for $\bar{a}(t)$ will not be bounded. This requirement is met if D is positive-definite [7].

Nonlinear programming cannot be used here in the minimization, as this requires constraints to be formulated in the form $g(D_{ij}) \le 0$ (g is a function of the elements of D). It is virtually impossible to pass from the condition of positive definiteness to constraints of that type for problems of dimensions $n \ge 3$.

To minimize the functional for positive-definite D, one needs special numerical methods that incorporate the detailed features, one of which is as follows.

Any matrix D can be uniquely represented as the sum of a symmetrical matrix D_s and an oblique-symmetric one D_o [7]: $D = D_s + D_o$, where $D_s = (D + D^*)/2$, $D_o = (D - D^*)/2$. Then D will be positive-definite if and only if D_s is so.

Then one minimizes f on the set of positive-definite D [8] in the following steps:

1) for certain z from the Euclidean space E^N ($N = (n-1)(n-2)/2$) and $\lambda \in E^{n-1}$ one constructs a mapping $D_s(z,\ \lambda)$ such as to take values on the set of symmetrical positive-definite matrices, where for any matrix D_s^0 one also finds z^0 and λ^0 such that $D_s(z^0,\ \lambda^0) = D_s^0$;

2) for $x \in E^N$, one constructs a mapping $D_o(x)$ that takes values on the set of oblique-symmetric matrices; and

3) methods of unconditional minimization with respect to the variables z, λ, and x are applied to $f[D_s(z,\ \lambda) + D_o(x)]$.

Let $\varepsilon > 0$ and Λ be a diagonal matrix having elements $\varepsilon + \lambda_i^2$ ($i = 1, 2, \ldots, n-1$) that are components of the vector $\lambda \in E^{n-1}$. A method has been described [8] by means of which any N-dimensional vector z is put into correspondence with an orthogonal matrix U(z). We put $D_s(z,\ \lambda) = U^*(z)\Lambda U(z)$.

We locate the elements of the N-dimensional vector x at points under the principal diagonal of D_o and these elements with minus signs above the principal diagonal to get a parametric representation of the set of oblique-symmetric matrices $D_o(x)$ with zero principal diagonal.

Then f(D) takes the form

$$f(D) = f[U^*(z)\Lambda U(z) + D_o(x)],$$

and the minimization is performed in the space of variables (z, λ, x) of dimensions $(n-1)^2$, where no constraints are imposed on the variables.

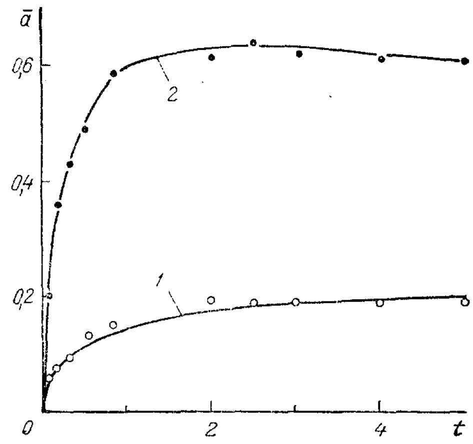

Fig. 1. Dependence of $\bar{a}$ (mole/kg) on time t (h) for adsorption of a mixture of isobutanol (1) and dimethylacetamide (2) from aqueous solution on particles of active anthracite (a_{01} = 0.21, a_{02} = 0.60 mole/kg).

This problem may be ill-posed [9, 10] in the sense that there may be several different points (z_*, λ_*, x_*) at which the function attains a minimum when small changes are made in the initial data; Tikhonov's regularization method can be applied, which involves minimization with a certain accuracy ε_k at each step for the function $T_k(z, \lambda, x) = f[D(z, \lambda, x)] + \alpha_k\Omega(z, \lambda, x)$, $\alpha_k > 0$, where $\Omega(z, \lambda, x) = \|z - z_0\|^2 + \|\lambda - \lambda_0\|^2 + \|x - x_0\|^2$; the matching of the parameters $_k$ and $_k$, which tend to zero, has been described in [10]. Then any sequence (z_k, λ_k, x_k) will have limiting points most remote from (z_0, λ_0, x_0) among all the (z_*, λ_*, x_*) on which f attains a minimum, which provides a stable determination of the solution (z_*, λ_*, x_*).

This approach is readily extended to the case where the function is dependent on two positive-definite matrices. This minimization method can also be used to solve other inverse problems in nonstationary mass transfer.

The metbod has been implemented on calculating the elements of the diffusion-coefficient matrix for a solid phase in the adsorption of a mixture of isobutanol (first component) and dimethylacetamide (second component) from aqueous solution onto activated anthracite having an equivalent radius for spherical particles of $0.282 \cdot 10^{-3}$ m. The calculations gave the following elements for matrix D: $D_{11} = 1.613 \cdot 10^{-12}$, $D_{12} = 0.490 \cdot 10^{-12}$, $D_{21} = 4.132 \cdot 10^{-12}$, $D_{22} = 3.312 \cdot 10^{-12}$ m²/sec. The diffusion-coefficient matrix has simple positive eigenvalues for these D_{ij}, and the transport within the solid in the adsorbed state causes an increase in entropy. These D_{ij} have been used with (3) to calculate the kinetic curves. The good match to experiment (Fig. 1) indicates that the D_{ij} can be determined in this way with an acceptable accuracy. The calculations show that small changes in $\bar{a}_i(t)$ (within the experimental error) do not give rise to substantially differing elements for D in the case n = 3.

These D_{ij} show that kinetic interaction on transport within a solid is quite pronounced, since the cross diffusion coefficients are of the same order as the principal ones, which must be borne in mind in models for sorption kinetics and dynamics for multicomponent mixtures involving mass transfer by diffusion.

NOTATION

j, mass flow density vector; D, square $(n - 1) \times (n - 1)$ matrix for diffusion in solid phase; n, number of components; a, component-concentration vector; x, coordinate; Γ, constant: for an infinite plate Γ = 0, infinite cylinder, Γ = 1, for a sphere Γ = 2; a_0, equilibrium-concentration vector; R, radius or half of plate thickness; I, unit matrix; q, number of measurements; D*, transposed matrix D of dimensions $(n - 1) \times (n - 1)$; Λ, diagonal matrix; U, orthogonal $(n - 1) \times (n - 1)$ matrix.

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THERMOELASTIC DEFORMATION OF A COOLED METAL PLATE UNDER THE INFLUENCE OF A PULSE-PERIODIC RADIATION FLUX

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A solution to the problem of determining the fields of stress and deformation in a plate under the influence of radiation flux with a Gaussian distribution is obtained.

A common element in optical systems is a metal plate, the surface of which has a high coefficient of reflection as a result of processing. Under the influence of a sufficiently high radiation flux density on the plate, the planar reflecting surface buckles due to nonuniform heating. This leads to a change in the structure of the beam; in particular, defocusing occurs as a result of reflection from such a surface [1]. In addition, thermal stress develops in the plate. During intense heating the magnitude of this stress can exceed the tensile strength of the plate material, thereby inducing an irreversible structural change.

In [2] a calculation of the thermal stress in a cooled plate under the influence of a pulse-periodic radiation flux was performed within a one-dimensional approximation where the stress tensor components and temperature change in the direction normal to the surface of the plate. In [3] a relation for the temperature fields in a plate was obtained within the one-dimensional approximation, and an estimation of the normal deformation and stress was performed. In [4] the two-dimensional problem of stress location in a free round plate under a radially Gaussian distributed radiation flux density was determined. It was shown that the structure of the spatial distribution of the stress within the one- and two-dimensional cases differs significantly. In particular, it was found that in the center zone of irradiation, the tangential and axial components of the stress are compressing, but out of the zone of irradiation they are stretching.

In the present work, in contrast to [4], the primary emphasis is the deformation of the plate surface induced by the thermal effect of a pulse-periodic radiation flux with a radial Gaussian distribution. We will assume that the rear surface of the plate is fixed to a rigid base, and the heat transfer from it proceeds according to Newton's law.

We will find the temperature field of a plate of constant thickness d and infinite in the radial direction. One of the surfaces of the plate ($z = 0$) is heated as a result of the influence of the pulse-periodic source (radiation directed along the normal to the surface), and the other ($z = d$) is cooled by means of a cooling agent with a coefficient of heat transfer h. We will assume that the intensity of the surface thermal source can be represented in the form

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