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MATHEMATICAL MODELING OF THE MOTION OF A PORTION OF HELIUM UNDER PULSED INJECTION OVER A FIXED BED OF CENOSPHERES

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A mathematical model is constructed and an analytical solution is obtained for the problem of a one-dimensional steady flow of a mixture of different gases with hollow permeable particles. The case of a one-dimensional unsteady flow of such a mixture is analyzed numerically. The numerical solutions are compared with experimental data on the motion of the peak concentration of helium in a fixed bed filled with cenospheres (solid hollow permeable spherical particles). The permeability of cenosphere walls and the drag coefficient of cenospheres in the gas flow are determined.

Key words: *mechanics of multiphase media, mathematical modeling, separation of gases.*

INTRODUCTION

In describing a system with a large number of particles, it is normally impossible to trace the motion of each particle, because it complicates the mathematical formulation of the problem. Various methods are used to reduce the number of independent variables, in particular, the probabilistic approach used in statistical physics. This approach implies that there is a function taking into account the probability of particle residence at certain points of space and the velocity of their motion, which allows correct averaging in space and time and obtaining the basic conservation laws thereby.

Another (phenomenological) approach is based on averaging the main parameters in time and space. The use of such a method is justified if the integral characteristics of the system rather than the characteristics of each particle are determined.

We consider a system consisting of a mixture of gases and containing solid hollow spherical particles (further called cenospheres), one of the gases being capable of penetrating into the cenospheres and going out of them. A model of such a system within the framework of mechanics of multiphase media is constructed, e.g., in [1] with the use of an approach proposed in [2]. Deriving of equations is based on the theory of interpenetrating continua, which implies that each continuum (our problem involves four continua: two for the gases outside the cenospheres, one for the permeable cenospheres, and one for the gas in the cenospheres) is described by its own parameters, which are integral characteristics of the original system.

The following assumptions were used in deriving the mathematical model:

1) the size of the solid particles is much greater than the mean free path in each gas and much smaller than the characteristic length of changing of macroscopic parameters;

2) cenospheres are hollow spherical particles of an identical diameter with a thin wall and have identical physical properties;

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3) one of the gases can penetrate inside the cenospheres; hence, the mass flow rate of this gas through the cenosphere shell is proportional to the difference in pressure inside and outside the shell;

4) the velocities and temperatures of the carrier gases outside the cenospheres coincide with each other;

5) the velocities and temperatures of the cenosphere shell and the gas inside the cenospheres are identical;

6) the gases are assumed to be ideal;

7) all parameters inside the cenospheres are uniform.

Using the approach developed in [2], we can write the system of equations

$$
\begin{gathered}
\frac{\partial \rho_{11}}{\partial t} + \operatorname{div}(\rho_{11}\boldsymbol{v}_1) = -K, \qquad \frac{\partial \rho_{12}}{\partial t} + \operatorname{div}(\rho_{12}\boldsymbol{v}_1) = 0, \\
\frac{\partial \rho_{21}}{\partial t} + \operatorname{div}(\rho_{21}\boldsymbol{v}_2) = K, \qquad \frac{\partial \rho_{22}}{\partial t} + \operatorname{div}(\rho_{22}\boldsymbol{v}_2) = 0, \\
\frac{\partial \rho_1\boldsymbol{v}_1}{\partial t} + \operatorname{div}(\rho_1\boldsymbol{v}_1 \times \boldsymbol{v}_1 + m_1 p I) = p\nabla m_1 - \boldsymbol{f}_{12} - K\boldsymbol{v}_2, \\
\frac{\partial \rho_2\boldsymbol{v}_2}{\partial t} + \operatorname{div}(\rho_2\boldsymbol{v}_2 \times \boldsymbol{v}_2 + m_2 p I) = p\nabla m_2 + \boldsymbol{f}_{12} + K\boldsymbol{v}_2, \\
\frac{\partial U_1}{\partial t} + \operatorname{div}[(U_1 + m_1 p)\boldsymbol{v}_1] = -q_{12}m_2 - \boldsymbol{f}_{12}\cdot\boldsymbol{v}_2 - K\Big(\varepsilon_2 + \frac{\boldsymbol{v}_2^2}{2}\Big) - p\,\frac{\partial m_1}{\partial t}, \\
\frac{\partial U_2}{\partial t} + \operatorname{div}[(U_2 + m_2 p)\boldsymbol{v}_2] = q_{12}m_2 + \boldsymbol{f}_{12}\cdot\boldsymbol{v}_2 + K\Big(\varepsilon_2 + \frac{\boldsymbol{v}_2^2}{2}\Big) - p\,\frac{\partial m_2}{\partial t}
\end{gathered}
\tag{1}
$$

with the closing relations

$$
\rho_1\varepsilon_1 = (\rho_{11}C_{11} + \rho_{12}C_{12})T_1, \qquad \rho_2\varepsilon_2 = (\rho_{21}C_{11} + \rho_{22}C_s)T_2,
$$

$$
m_1 + m_2 = 1, \qquad \rho_{22} = \rho_{22}^0(1 - \beta^3)m_2.
$$

Hereinafter,

$$
p_{11} = \frac{\rho_{11}R_1T_1}{m_1}, \qquad p_{12} = \frac{\rho_{12}R_2T_1}{m_1}, \qquad p_{21} = \frac{\rho_{21}R_1T_2}{m_2}\,\beta^3,
$$

$$
U_1 = \rho_1(\varepsilon_1 + \boldsymbol{v}_1^2/2), \qquad U_2 = \rho_2(\varepsilon_2 + \boldsymbol{v}_2^2/2),
$$

$$
\rho_1 = \rho_{11} + \rho_{12}, \qquad \rho_2 = \rho_{21} + \rho_{22}, \qquad p = p_{11} + p_{12},
$$

$$
K = C_m(p_{11} - p_{21})m_2, \qquad \boldsymbol{f}_{12} = C_F\,\frac{m_2}{m_1}\,\frac{1}{R^2}\,(\rho_{11}\nu_1 + \rho_{12}\nu_2)(\boldsymbol{v}_1 - \boldsymbol{v}_2),
$$

$$
\beta = r/R,
$$

t is the time, I is the unit tensor, ρ_{11} is the density of the gas capable of penetrating into the cenospheres, averaged over the volume outside the cenospheres, ρ_{12} is the density of the gas that cannot penetrate into the cenospheres, averaged over the volume outside the cenospheres, ρ_{21} is the volume-averaged density of the gas in the cenospheres, ρ_{22} is the volume-averaged density of the cenosphere shell, $\boldsymbol{v}_1$ is the velocity of gas motion outside the cenospheres, $\boldsymbol{v}_2$ is the velocity of cenosphere motion, T_1 is the gas temperature outside the cenospheres, T_2 is the temperature of the cenospheres and the gas inside the cenospheres, m_1 is the volume concentration of the gas outside the cenospheres, m_2 is the volume concentration of the cenospheres, ε_1 and ε_2 are the specific internal energies of the first and second continua, respectively, ρ_{22}^0 is the density of the cenosphere materials, r is the radius of the inner cavity of the cenosphere, R is the cenosphere radius, C_m is the permeability of the cenospheres, C_F is the drag coefficient of the cenospheres in the gas flow, q_{12} is the heat flux between the phases, C_{11} and C_{12} are the thermal conductivities of the gases capable and incapable of penetrating into the cenospheres, C_s is the thermal conductivity of the solid material of the cenospheres, and ν_1 and ν_2 are the viscosities of the gases capable and incapable of penetrating into the cenospheres, respectively.

System (1) is similar to the famous Euler equations. The difference lies in the right sides that take into account the redistribution of mass, momentum, and energy between the continua. It should be noted that viscosity is only used in determining the forces of interaction between the continua of the gas and cenospheres. In the general case, the quantities C_m and C_F are variable and are functions of other parameters of the medium, but they may be assumed to be constant for a qualitative analysis of the phenomenon.

1. ONE-DIMENSIONAL UNSTEADY MOTION

1.1. Mathematical Model. The mathematical model of this problem follows from the general system of equations. The following additional assumptions are used: the motion is one-dimensional and unsteady, $m_2 = 1 - m_1 = \text{const}$, $v_2 = 0$, and $T_1 = T_2 = T = \text{const}$. In the general case, these expressions cannot be substituted into the original system, because the cenospheres are initially in a suspended state. In the problem posed, they are fixed and motionless; therefore, we use only the laws of conservation of mass and momentum for the gas outside the cenospheres from the original model. As a result, we obtain the following closed system of differential equations:

$$\rho_{21,t} = C_m(p_{11} - p_{21})m_2,$$
$$\rho_{11,t} + (\rho_{11}v_1)_x = -C_m(p_{11} - p_{21})m_2, \qquad \rho_{12,t} + (\rho_{12}v_1)_x = 0, \tag{2}$$
$$(\rho_1 v_1)_t + (\rho_1 v_1^2 + P)_x = -C_F \frac{m_2}{m_1} \frac{1}{R_+^2} (\rho_{11}\nu_1 + \rho_{12}\nu_2)v_1.$$

Here

$$p_{11} = \rho_{11}R_1T/m_1, \qquad p_{21} = \rho_{21}R_1T/(\beta^3 m_2), \qquad P = \rho_{11}R_1T + \rho_{12}R_2T,$$
$$m_1 + m_2 = 1, \qquad \rho_1 = \rho_{11} + \rho_{12},$$

ρ_{21} is the density of helium that entered the cenospheres, ρ_{11} is the density of helium outside the cenospheres, ρ_{12} is the density of the gas outside the cenospheres, the physical parameters of the gas being essentially different from helium parameters, v_1 is the velocity of motion of the mixture, m_2 is the volume concentration of cenospheres, R_1 and R_2 are the gas constants (the subscripts 1 and 2 refer to helium and the other gas), T is the temperature, ν_1 and ν_2 are the viscosities of the gases, and R_+ is the outer radius of the cenospheres.

1.2. Characteristics of the Mathematical Model. We determine the type of the mathematical model (2). Developing the derivatives, we pass to the following system of differential equations:

$$\rho_{21,t} = K, \qquad \rho_{11,t} + v_1\rho_{11,x} + \rho_{11}v_{1,x} = -K, \qquad \rho_{12,t} + v_1\rho_{12,x} + \rho_{12}v_{1,x} = 0,$$
$$v_{1,t} + \frac{1}{\rho_1} P_x + v_1 v_{1,x} = \Big(K - C_F \frac{m_2}{m_1} \frac{1}{R_+^2} (\rho_{11}\nu_1 + \rho_{12}\nu_2)\Big)\frac{v_1}{\rho_1}. \tag{3}$$

Here

$$K = C_m m_2\Big(\frac{\rho_{11}}{m_1} - \frac{\rho_{21}}{\beta^3 m_2}\Big)R_1T, \qquad \rho_1 = \rho_{11} + \rho_{12}, \qquad P = \rho_{11}R_1T + \rho_{12}R_2T.$$

Thus, the system can be presented as

$$U_t + A(U)U_x = R(U),$$

where

$$U = \begin{pmatrix} \rho_{21} \\ \rho_{11} \\ \rho_{12} \\ v_1 \end{pmatrix}, \qquad A = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & v_1 & 0 & \rho_{11} \\ 0 & 0 & v_1 & \rho_{12} \\ 0 & R_1T/\rho_1 & R_2T/\rho_1 & v_1 \end{pmatrix},$$

$$R = \begin{pmatrix} K \\ -K \\ 0 \\ \Big(K - C_F \dfrac{m_2}{m_1} \dfrac{\rho_{11}\nu_1 + \rho_{12}\nu_2}{R_+^2}\Big)\dfrac{v_1}{\rho_1} \end{pmatrix}.$$

We find the Jordan expansion of the matrix A:

$$A = rdl \qquad (l = r^{-1}).$$

The eigenvalues are 0, v_1, $v_1 - c$, and $v_1 + c$ ($c = \sqrt{P/\rho_1}$ is an analog of the velocity of sound for the mixture as a whole).

The sought expressions for r and l have the form

$$r = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -\dfrac{R_2}{R_1} & -\dfrac{\rho_{11}}{c} & \dfrac{\rho_{11}}{c} \\ 0 & 1 & -\dfrac{\rho_{12}}{c} & \dfrac{\rho_{12}}{c} \\ 0 & 0 & 1 & 1 \end{pmatrix}, \qquad l = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -\dfrac{R_1\rho_{12}}{R_1\rho_{11}+R_2\rho_{12}} & \dfrac{R_1\rho_{11}}{R_1\rho_{11}+R_2\rho_{12}} & 0 \\ 0 & -\dfrac{R_1T}{2\sqrt{\rho_1 P}} & -\dfrac{R_2T}{2\sqrt{\rho_1 P}} & \dfrac{1}{2} \\ 0 & \dfrac{R_1T}{2\sqrt{\rho_1 P}} & \dfrac{R_2T}{2\sqrt{\rho_1 P}} & \dfrac{1}{2} \end{pmatrix}.$$

In the case considered, the flow velocity is low ($v_1 < c$), and the motion is assumed to be unidirectional. Hence, there are two positive characteristics, one negative characteristic, and one zero characteristic. Thus, system (3) is hyperbolic, though the full system (1) is presumably of a composite type [2].

2. ONE-DIMENSIONAL STEADY MOTION

2.1. Mathematical Model. In a steady-state case, the system is written as

$$p_{11} = p_{21}, \qquad (\rho_{11}v_1)_x = 0, \qquad (\rho_{12}v_1)_x = 0,$$
$$(\rho_1 v_1^2 + \rho_{11}R_1T + \rho_{12}R_2T)_x = -C_F\,\frac{m_2}{m_1}\,\frac{1}{R_+^2}\,(\nu_1\rho_{11} + \nu_2\rho_{12})v_1. \tag{4}$$

The solution of Eqs. (4) is sought for

$$\rho_{11}\Big|_{x=0} = \rho_{11}^0, \qquad \rho_{12}\Big|_{x=0} = \rho_{12}^0, \qquad v_1\Big|_{x=0} = v_1^0.$$

Here ρ_{11}^0, ρ_{12}^0, and v_1^0 are the densities and flow velocity at the point $x = 0$.

The case with $x > 0$ and $v_1^0 > 0$ is of interest for the further study, and the solution for $v_1^0 < 0$ is readily obtained from the previous solution.

2.2. Qualitative Analysis of the Problem. In a steady case, the first integrals of system (4) have the form

$$\rho_{11}v_1 = C_1, \qquad \rho_{12}v_1 = C_2,$$
$$\alpha_0 v_1 + \frac{\alpha_R T}{v_1} = -C_F\,\frac{m_2}{m_1}\,\frac{1}{R_+^2}\,\alpha_\nu x + C_3.$$

Here $\alpha_0 = C_1 + C_2$, $\alpha_R = C_1R_1 + C_2R_2$, $\alpha_\nu = C_1\nu_1 + C_2\nu_2$, C_1, C_2, and C_3 are constants:

$$C_1 = \rho_{11}^0 v_1^0, \quad C_2 = \rho_{11}^0 v_1^0, \quad C_3 = (\rho_{11}^0 + \rho_{12}^0)(v_1^0)^2 + (\rho_{11}^0 R_1 + \rho_{12}^0 R_2)T.$$

The relation $p_{11} = p_{21}$ yields

$$\rho_{21} = \beta^3 m_2 \rho_{11}/m_1.$$

Let us demonstrate how this system with initial conditions can yield the solution of the Cauchy problem, written in explicit form, and also indicate the mathematical criterion of solubility of this system in the case of a finite length of the examined region (e.g., in the case of motion of a mixture of gases through a fixed bed filled with cenospheres).

We write the law of conservation of momentum in a form most convenient for the further study:

$$\alpha_0(v_1 - v_1^0) + \alpha_R T(1/v_1 - 1/v_1^0) = -C_F'\alpha_\nu x$$

[$C_F' = C_F(m_2/m_1)/R_+^2$]. This relation is an implicit dependence $v_1(x)$. An explicit relation is obtained by solving the quadratic equation with respect to v_1. Another method of deriving this dependence is described below, which allows a more detailed study of the flow.

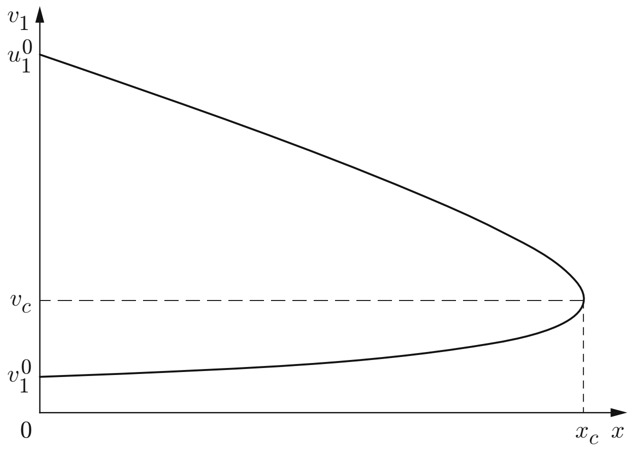

Fig. 1

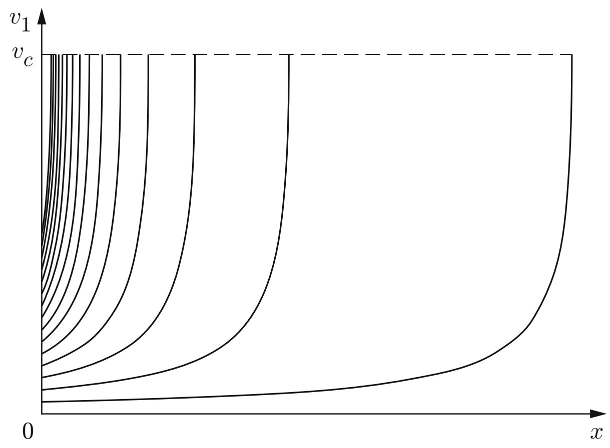

Fig. 2

Fig. 1. Dependence $v_1(x)$.

Fig. 2. Qualitative behavior of the subsonic branch of the dependence $v_1(x)$ for initial velocities $v_1^0 = v_1(0) < v_c$ for one composition of the mixture.

Based on the above-given equation, we express x as a function of v_1:

$$x = f(v_1) = -\frac{1}{C'_F\alpha_\nu}\Big[\alpha_0(v_1 - v_1^0) + \alpha_R T\Big(\frac{1}{v_1} - \frac{1}{v_1^0}\Big)\Big].$$

We check whether the function f has extreme points, i.e., $\partial f/\partial v_1 = 0$ if and only if

$$v_1 = v_c = \sqrt{\frac{\alpha_R T}{\alpha_0}} = \sqrt{\frac{p_0}{\rho_1^0}} = \sqrt{\frac{\rho_{11}}{\rho_{11}+\rho_{12}}\,R_1T + \frac{\rho_{12}}{\rho_{11}+\rho_{12}}\,R_2T}$$

(p_0 and ρ_1^0 are the pressure and the total density of the mixture of gases at the bed entrance). Note that the constant quantity v_c remaining unchanged along the bed is an analog of the velocity of sound for this mixture of gases.

The following estimate can be readily obtained for v_c. Let $c_1 = \sqrt{R_1T}$ and $c_2 = \sqrt{R_2T}$ be the velocities of sound for the two gases used in the mixture. (We assume that $c_1 < c_2$; otherwise, the signs should be changed to the opposite ones.) Hence, the following relation is valid:

$$c_1 \le v_c \le c_2.$$

The closeness of the value of v_c to one of the values of c_i $(i = 1, 2)$ depends on the initial composition of the mixture.

The qualitative dependence $v_1(x)$ is plotted in Fig. 1. Two types of flow are seen to be formed: 1) subsonic flow for $v_1\Big|_{x=0} = v_1^0 < v_c$; 2) supersonic flow for $v_1\Big|_{x=0} = u_1^0 > v_c$. The second case is unphysical, because it describes gas exhaustion from a region with a lower pressure to a region with a higher pressure (it follows from the relation $\rho_{11}v_1 = C_1$ and the pressure–density relation for an ideal gas).

In what follows, we consider mixtures with specified values of ρ_{11}^0 and ρ_{12}^0. Figure 2 shows the flow pattern for one composition of the mixture with different initial velocities v_1^0.

For a prescribed initial composition of the mixture and velocities of gases at the bed entrance, we formulate the condition of existence of the solution of a one-dimensional steady-state problem on passing of the gas mixture through a fixed bed of cenospheres located on the segment $[0, L]$. It follows from Fig. 1 that such a flow is "blocked" at the critical point $x = x_c$. Thus, the criterion of existence of the steady-state solution has the form

$$x_c = f(v_c) \ge L.$$

Substituting f into this expression, we obtain the inequality

$$|v_1^0 - v_c| \ge \sqrt{C'_F\alpha_\nu L v_1^0/\alpha_0}.$$

3. SOLUTION OF THE PROBLEM OF MOTION OF THE HELIUM CONCENTRATION PEAK THROUGH A FIXED BED

Let us consider the following physical problem for verification of the mathematical model derived. A fixed bed is filled with cenospheres, and an argon flow is initiated through the bed. Helium is supplied in a pulsed manner to the bed entrance and is entrained by the argon flow in the downstream direction. In contrast to argon, helium can easily penetrate into the cenospheres and leave them. The solution of this problem is necessary not only to verify the mathematical model and refine some constants in the governing equations, but also to elucidate the possibility of using cenospheres as a filter in the process of mixture enrichment by helium.

The equations that describe the motion of the gases in the fixed bed are given in Sec. 1. To integrate system (3) numerically, we need to impose the initial and boundary conditions.

3.1. Initial Conditions. Let us assume that helium is not jet injected into the bed. In this case, the bed filled with cenospheres contains a steady flow of the carrier gas, which is not adsorbed by these cenospheres. Let us determine the profiles of velocity and density in the flow, based on the known gas pressure at the entrance and exit of the fixed bed. In this case, system (4) acquires the form

$$(\rho_{12}v_1)_x = 0,$$
$$(\rho_{12}v_1^2 + \rho_{12}R_2T)_x = -C_F\,\frac{m_2\nu_2}{m_1}\,\frac{1}{R_+^2}\,\rho_{12}v_1, \tag{5}$$

where $v_1(x)$ and $\rho_{12}(x)$ are the sought functions.

The boundary conditions are

$$\rho_{12}\Big|_{x=0} = \frac{p_0}{R_2T}, \qquad \rho_{12}\Big|_{x=L} = \frac{p_a}{R_2T}, \qquad p_a < p_0,$$

where p_0 and p_a are the prescribed pressures at the bed entrance and exit, respectively.

Based on the volume gas flux F at the bed exit, we can determine the drag coefficient of the medium C_F. Let T_a be the ambient temperature, p_a be the atmospheric pressure, and S be the cross-sectional area of the fixed bed. Then

$$p_a = \rho_{12}v_1SR_2T_a/F.$$

Integrating the equations of the original system (5) with respect to x, we obtain

$$\rho_{12}v_1 = \rho_{12}^0v_1^0,$$
$$\rho_{12}^0v_1^0(v_1 - v_1^0) + R_2T(\rho_{12} - \rho_{12}^0) = -C_F\,\frac{m_2}{m_1}\,\frac{\nu_2}{R_+^2}\,\rho_{12}^0v_1^0x.$$

Here ρ_{12}^0 and v_1^0 are the density and velocity at $x = 0$.

It follows from the boundary conditions that

$$\rho_{12}^0 = p_0/(R_2T),$$

and the relation for the flow at the bed exit and the first integral yield the expression

$$\rho_{12}v_1 = \rho_{12}^0v_1^0 = \rho_{12}^Lv_1^L = p_aF/(SR_2T_a),$$

where $\rho_{12}(L) = \rho_{12}^L$ and $v_1(L) = v_1^L$. Hence, we obtain

$$v_1^0 = p_aTF/(p_0T_aS).$$

Similarly, the velocity at the bed exit is described by

$$v_1^L = TF/(T_aS).$$

From the second integral of system (5), we express C_F through the known values of ρ_{12} and v_1 at the domain boundaries:

$$C_F = \frac{m_1R_+^2}{m_2\nu_2L}\Big[\frac{T}{T_a}\,\frac{F}{S}\Big(\frac{p_a}{p_0} - 1\Big) + R_2T_a\,\frac{S}{F}\Big(\frac{p_0}{p_a} - 1\Big)\Big]. \tag{6}$$

To obtain the values of the sought functions in the entire domain of motion, we have to resolve the second integral of system (5) with the use of the dependences obtained. As a result, we obtain the equation for v_1:

$$v_1^2 + \Big\{\frac{T}{T_a}\,\frac{F}{S}\Big[\frac{x}{L}\Big(\frac{p_a}{p_0} - 1\Big) - \frac{p_a}{p_0}\Big] + R_2 T_a\,\frac{S}{F}\Big[\frac{x}{L}\Big(\frac{p_0}{p_a} - 1\Big) - \frac{p_0}{p_a}\Big]\Big\} v_1 + R_2 T = 0.$$

The first integral of system (5) yields

$$\rho_{12} = p_a F/(S R_2 T_a v_1).$$

Thus, knowing all initial data, we can obtain the initial velocity and density profiles.

3.2. Boundary Conditions. Let helium be supplied in a pulse at the time $t = 0$. In accordance with the analysis in Sec. 1, the boundary-value problem has to be subjected to the initial condition at $t = 0$, two conditions on the left boundary $x = 0$, and one condition on the right boundary $x = L$. In this case, we set the conditions for pressure:

$$p_{11}\Big|_{x=0} = \begin{cases} p_0, & t \le t_c, \\ 0, & t > t_c, \end{cases} \qquad p_{12}\Big|_{x=0} = \begin{cases} 0, & t \le t_c, \\ p_0, & t > t_c, \end{cases} \qquad p_{11} + p_{12}\Big|_{x=L} = p_L.$$

Here p_{11} is the helium pressure outside the cenospheres, p_{12} is the pressure of the carrier gas, p_0 is the carrier gas pressure prescribed at the bed entrance, and p_L is the pressure at the bed exit.

3.3. Numerical Integration of the Problem. We define two uniform grids on the segment $[0, L]$: with values in integer nodes $\omega_h^1 = \{x_0 = 0,\ x_1 = h,\ \ldots,\ x_N = L\}$ and with values in fractional nodes $\omega_h^2 = \{x_{1/2} = h/2,\ x_{3/2} = 3h/2,\ \ldots,\ x_{N-1/2} = L - h/2\}$ (h is the step of the difference grid).

The functions ρ_{21}, ρ_{11}, and ρ_{12} are projected onto the grid ω_h^2, and the function v_1 is projected onto the grid ω_h^1.

The original differential equations, except for the equation

$$\rho_{21,t} = C_m R_1 T (m_2 \rho_{11}/m_1 - \rho_{21}/\beta^3),$$

can be written as

$$\frac{\partial U}{\partial t} + A(U)\,\frac{\partial U}{\partial x} = R(U).$$

Here

$$U = \begin{pmatrix} \rho_{11} \\ \rho_{12} \\ v_1 \end{pmatrix}, \qquad A(U) = \begin{pmatrix} v_1 & 0 & \rho_{11} \\ 0 & v_1 & \rho_{12} \\ R_1 T/\rho_1 & R_2 T/\rho_1 & v_1 \end{pmatrix},$$

$$R = \begin{pmatrix} -K \\ 0 \\ \Big(K - C_F\,\dfrac{m_2}{m_1}\,\dfrac{\rho_{11}\nu_1 + \rho_{12}\nu_2}{R_+^2}\Big)\dfrac{v_1}{\rho_1} \end{pmatrix}$$

$[K = C_m R_1 T (m_2 \rho_{11}/m_1 - \rho_{21}/\beta^3)]$.

We identify the diagonal part in the matrix at the derivative with respect to x, i.e., we present the matrix as the sum

$$A(U) = B(U) + v_1 I'$$

(I' is a unit matrix of dimension 3×3). The numerical solution is sought as follows. At the first stage, we solve the problem $\partial U/\partial t = G$ ($G = R(U) - B(U)\,\partial U/\partial x$), where we find the values of the quantities at the intermediate stage. At the second stage, we solve the problem $\partial U/\partial t + v_1\,\partial U/\partial x = 0$, where the values at the next time layer are obtained through the values at the intermediate stage.

At the first stage, we have

$$\frac{\rho^*_{21,j+1/2} - \rho^n_{21,j+1/2}}{\tau} = K^n_{j+1/2},$$

$$\frac{\rho^*_{11,j+1/2} - \rho^n_{11,j+1/2}}{\tau} = -K^n_{j+1/2} - \rho^n_{11,j+1/2}\,\frac{v^n_{1,j+1} - v^n_{1,j}}{h},$$

$$\frac{\rho^*_{12,j+1/2} - \rho^n_{12,j+1/2}}{\tau} = -\rho^n_{12,j+1/2} \frac{v^n_{1,j+1} - v^n_{1,j}}{h},$$

$$\frac{v^*_{1,j} - v^n_{1,j}}{\tau} = f^n_j - \frac{2T}{\rho^n_{1,j+1/2} + \rho^n_{1,j-1/2}} \Big(R_1 \frac{\rho^n_{11,j+1/2} - \rho^n_{11,j-1/2}}{h} + R_2 \frac{\rho^n_{12,j+1/2} - \rho^n_{12,j-1/2}}{h} \Big).$$

Here τ is the time step; the quantities marked by the superscript asterisk are parameters at the intermediate stage.

At the second stage, we obtain

$$\rho^{n+1}_{21,j+1/2} = \rho^*_{21,j+1/2},$$

$$\frac{\rho^{n+1}_{11,j+1/2} - \rho^*_{11,j+1/2}}{\tau} + \frac{v^*_{1,j} + v^*_{1,j+1}}{2} \frac{\rho^*_{11,j+1/2} - \rho^*_{11,j-1/2}}{h} = 0,$$

$$\frac{\rho^{n+1}_{12,j+1/2} - \rho^*_{12,j+1/2}}{\tau} + \frac{v^*_{1,j} + v^*_{1,j+1}}{2} \frac{\rho^*_{12,j+1/2} - \rho^*_{12,j-1/2}}{h} = 0,$$

$$\frac{v^{n+1}_{1,j} - v^*_{1,j}}{\tau} + v^*_{1,j} \frac{v^*_{1,j} - v^*_{1,j-1}}{h} = 0.$$

Here

$$K^n_{j+1/2} = C_m R_1 T \Big(\frac{m_2}{m_1} \rho^n_{11,j+1/2} - \frac{1}{\beta^3} \rho^n_{21,j+1/2} \Big), \qquad \rho_{1,j+1/2} = \rho_{11,j+1/2} + \rho_{12,j+1/2},$$

$$f^n_j = \Big[\frac{K^n_{j+1/2} + K^n_{j-1/2}}{2} - C_F \frac{m_2}{m_1} \frac{1}{R^2} \Big(\frac{\rho^n_{11,j+1/2} + \rho^n_{11,j-1/2}}{2} \nu_1 + \frac{\rho^n_{12,j+1/2} + \rho^n_{12,j-1/2}}{2} \nu_2 \Big) \Big] \frac{2v^n_{1,j}}{\rho^n_{1,j+1/2} + \rho^n_{1,j-1/2}}.$$

3.4. Results of the Numerical Experiment. The numerical experiment was performed for a fixed bed 1 m long with an inner diameter of 3 mm, which was filled with spherical particles (cenospheres) of radius of 80 μm (the ratio of the inner to the outer radius was 0.91; the volume concentration of cenospheres was 0.6). The carrier gas was argon, and its excess pressure at the bed entrance was 0.17 MPa; the gas pressure at the bed exit was assumed to have the atmospheric value. The bed temperature varied from 273 to 800 K, the volume flow rate of argon was approximately 0.476 cm^3/sec at room temperature and atmospheric pressure, and the mass of the helium portion was 0.2301 mg.

To compare the results of numerical and physical experiments, we determined the time evolution of the helium flow rate at the bed exit. In the computations, the initial profile of the helium concentration at the bed entrance was assumed to be rectangular.

Figure 3 shows the results calculated for a rectangular profile with different permeabilities C_m. With increasing C_m, the character of the dependence $M(t)$ becomes essentially different. For low permeabilities (Fig. 3a), a certain decrease in the maximum concentration and a typical pattern with a smeared rear front of the peak are observed. Such a character of the dependence $M(t)$ in the physical experiment corresponds to slow diffusion of helium inward the cenospheres at low temperatures or to a situation where the gas cannot penetrate inward the particles (e.g., nitrogen). As the permeability increases (Fig. 3b), the curves are shifted toward higher times, which is accompanied by strong smearing of the rear front of the peak. With a further increase in permeability, the maximum of the concentration is shifted toward higher times of gas confinement. At high rates of the diffusion process, the dependence $M(t)$ becomes almost symmetric; the width of the pulse becomes almost twice the time of confinement of the non-adsorbed species, which is determined by the ratio of the volume available for helium to the volume between the cenospheres (equal to 2.13). Such a behavior of the system agrees with the theory of the chromatographic process and is qualitatively consistent with the previous statistical calculations [3].

The calculated results were compared with experimental data obtained with a fraction of cenospheres 0.063 to 0.100 mm from the concentrate of fly ashes of the Moscow Cogeneration Plant No. 22 by the method of aerodynamic separation (the bulk density was 0.18 g/cm^3, the mean radius was 40 μM, and the calculated ratio of the inner to the outer radius was 0.978). The length of the layer of cenospheres in the fixed bed with an inner diameter of 3 mm was 1 m; the carrier gas was argon with a volume flow rate of 0.121 cm^3/sec ($T_a = 273$ K and $p_a = 0.1013$ MPa). The permeability was changed by varying the bed temperature in the range of 300 to 850 K. The excess pressure of

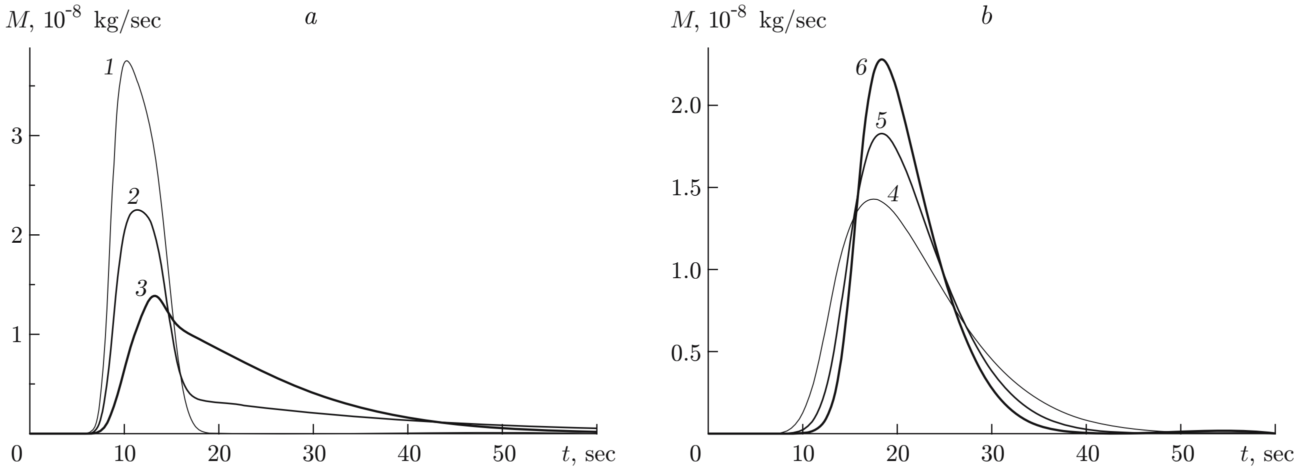

Fig. 3. Flow rate of helium at the bed exit for different permeabilities of the cenospheres C_m: $C_m = 0$ (1), 10^{-7} (2), $3 \cdot 10^{-7}$ (3), 10^{-6} (4), $5 \cdot 10^{-6}$ (5), and 10^{-5} sec/m^2 (6).

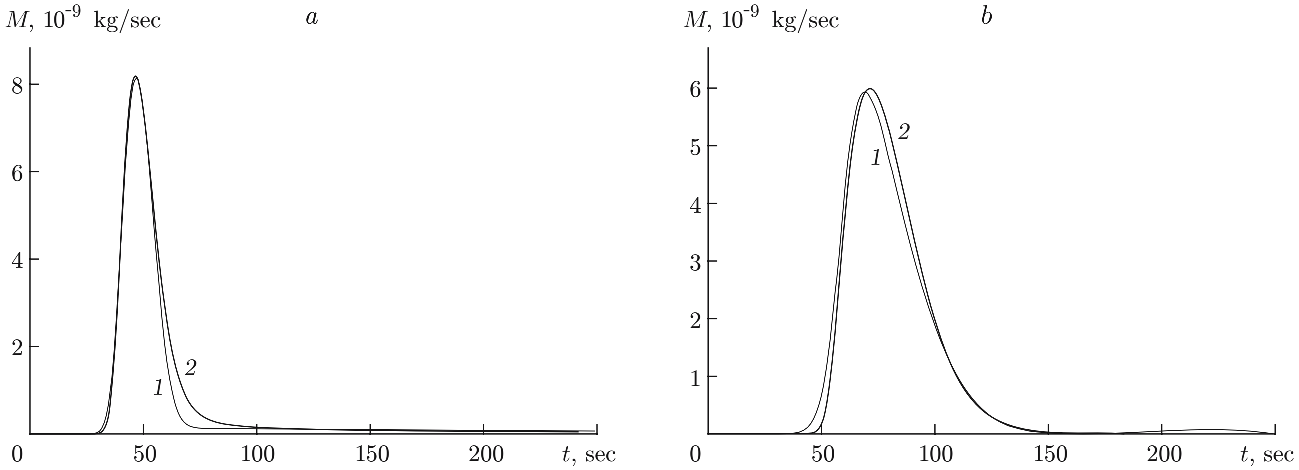

Fig. 4. Dependences $M(t)$ obtained in numerical calculations (1) and physical experiments (2) with $T = 216$ (a) and 580°C (b).

the carrier gas at the bed entrance was 0.06–0.17 MPa, and the gas pressure at the bed exit had the atmospheric value.

As a quantitative comparison of the model with experimental data requires fitting of system parameters (primarily, the permeability), it seems reasonable to perform the first comparisons in extreme cases, i.e., with very high and very low permeabilities. For intermediate values, the model is expected to give a satisfactory description of the system behavior. The dependences $M(t)$ obtained in numerical calculations and physical experiments are plotted in Fig. 4.

Comparisons of numerical and experimental data allow us to draw the following conclusions.

The model proposed offers an adequate description of the displacements of the peaks, the change in the peak width, and the evolution of the peak shape with variation of permeability.

The model gives a satisfactory description of the displacement of the helium peak with permeability varied from the minimum value (almost no diffusion) to the maximum value (close to equilibrium penetration of helium): the displacement of the helium peak in terms of time is approximately 9 sec in calculations and 10 sec in experiments (at $T = 216$ and 580°C).

The model ensures a satisfactory description of the general laws of the system behavior. A quantitative comparison of the calculated and experimental results allows determining the permeability of the cenosphere walls C_m and the drag coefficient of the cenosphere medium C_F [by Eq. (6)], which can be used for further calculations (in our case, $C_m = 5 \cdot 10^{-9}$ sec/m^2 and $C_F = 256.019$ for $T = 216$°C; $C_m = 3 \cdot 10^{-7}$ sec/m^2 and $C_F = 303.112$ for $T = 580$°C).

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