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THERMOPHORETIC MOTION OF AN ENSEMBLE OF MODERATELY COARSE AEROSOL PARTICLES

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Knowledge of the laws governing the behavior of an ensemble of aerosol particles in a nonisothermal gas makes it possible to increase the efficiency of many industrial operations (production of powders, removal of valuable or hazardous by-products from the atmosphere, etc.). Such knowledge can also be useful in developing both natural and artificial methods of influencing cloud formation and movement. The latter is important, for example, in the use of aerosols in agriculture.

The solution of thermophoresis problems entails calculation of the relative motion of a nonuniformly heated gas and aerosol particles suspended in it. The principal assumption underlying the hydrodynamic method of calculation proposed in [1] is that the particles are distant from one another and can each be regarded as an individual particle located in an infinite gas. Gaidukov and Melekhov [2] and Yalamov et al. [3] used this method to develop an approach which makes it possible to study the thermophoretic motion of an arbitrary collection of solid aerosol particles located close enough to one another to allow their hydrodynamic interaction. By hydrodynamic interaction, it is meant that the interaction is due to the fact that a particle moving in the medium generates a velocity field that affects the motion of other particles. By virtue of the assumptions made in the mathematical formulation of the problem, the results presented in [2, 3] are valid only for an ensemble con-

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sisting of identical coarse (Kn ≤ 0.05, Kn = λ/R, where λ is the mean free path of the gas molecules and R is the radius of the particles) and moderately heat-conducting particles.

In the present study, we generalize the approach taken in [2, 3] to the case of moderately coarse and high-heat-conducting particles. We use a computer to calculate the behavior of linear ensembles on the basis of expressions obtained for the steady-state velocity of each particle. We also study the effect of polydispersity on the process of particle coarsening.

We make the following assumptions: the gaseous medium is at rest far from the particles; the temperature of the medium is a linear function of position; the particles are solid and spherical (not necessarily of the same size) and are distributed randomly in space; at the initial moment of time, the particles have a steady velocity $u^{(k)}$ (k = 1, 2, ..., N).

The problem has two parts. First we need to find a correction for the thermophoretic velocity of a single moderately coarse aerosol particle. This correction depends on the parameters $h_{\alpha k} = R_\alpha/\ell_{\alpha k}$ (where R_α is the radius of a particle with the number α and $\ell_{\alpha k}$ is the distance between the centers of corresponding particles). In the second part of the problem, we need to calculate the trajectory of the particles.

Estimates [4] show that within the practicable range of temperature gradients, the fields of velocity, pressure, and temperature of the gaseous medium (v, p, T_e) are determined by the quasisteady Stokes equations and the Laplace equation [4]

$$\eta\nabla^2 v = \nabla P,\ \nabla v = 0; \tag{1}$$

$$\nabla^2 T_e = 0. \tag{2}$$

On the surface of each particle, the macroscopic parameters of the medium satisfy the following boundary conditions

$$v_{rk} = c_V \frac{\nu_e}{R_k^2 T_{e0}} \mathrm{Kn}^{(k)} \frac{1}{\sin\theta_k} \frac{\partial}{\partial\theta_k} \sin\theta_k \frac{\partial}{\partial\theta_k} T_e; \tag{3}$$

$$v_{\theta k} = K_{TS}^{(0)}\left(1 + \mathrm{Kn}^{(k)}\beta_R'\right) \frac{\nu_e}{R_k T_{e0}} \frac{\partial}{\partial\theta_k} T_e + \tag{4}$$

$$+ c_m R_k \mathrm{Kn}^{(k)} \Pi_{r_k\theta_k} + K_{TS}^{(0)} \mathrm{Kn}^{(k)} \beta_R \frac{\nu_e}{T_{e0}} \frac{\partial^2}{\partial\theta_k\,\partial r_k} T_e - K_{TS}^{(0)} \beta_b \mathrm{Kn}^{(k)} \frac{R_k \nu_e}{2T_{e0}} T_{r_k\theta_k};$$

$$\varkappa_e \frac{\partial T_e}{\partial r_k} - \varkappa_k \frac{\partial T_k}{\partial r_k} = c_q \varkappa_e \mathrm{Kn}^{(k)} \frac{1}{R_k \sin\theta_k} \frac{\partial}{\partial\theta_k} \sin\theta_k \frac{\partial}{\partial\theta_k} T_e; \tag{5}$$

$$T_e - T_k = K_T \mathrm{Kn}^{(k)} R_k (\partial T_e/\partial r_k) \tag{6}$$

$$\left(\Pi_{r_k\theta_k} = r_k \frac{\partial}{\partial r_k}\left(\frac{v_{ek}}{r_k}\right) + \frac{1}{r_k}\frac{\partial v_{rk}}{\partial\theta_k};\quad T_{r_k\theta_k} = r_k \frac{\partial}{\partial r_k}\left(\frac{1}{r_k^2}\frac{\partial T_e}{\partial\theta_k}\right) + \frac{1}{r_k}\frac{\partial^2 T_e}{\partial r_k\,\partial\theta_k}\right).$$

Here, $K_{TS}^{(0)}$, c_m are the thermal and isothermal slip coefficients of the gas along a plane surface; K_T is a coefficient expressing the temperature jump at the plane surface; $\nu_e = \eta_e/\rho_e$; η_e, $\varkappa_e$, ρ_e are the viscosity, thermal conductivity, and mass density of the gas; $\varkappa_k$ is the thermal conductivity of the substance of the k-th particle; the quantities c_V, β_R', β_R, β_b, c_q, entering into terms which are proportional to $\mathrm{Kn}^{(k)}$ and appear in boundary conditions (3)-(5) when allowance is made for the curvature of the surface and the Barnett contributions to the velocity distribution function of the gas molecules, are complex functions of the accommodation coefficients; r_k, θ_k, and φ_k is the spherical coordinate system connected with the k-th particle and having its origin at the center of the particle. We will use the expressions obtained in [5] for c_V, β_R', β_R, β_b, c_q.

Knowing the solution of Eqs. (1), (2) with boundary conditions (3)-(6), we can determine the total forces acting on each particle of the ensemble. Assuming the motion to be steady, we find the instantaneous velocities $u^{(k)}$ of the particles by equating the total forces to zero, while we find their trajectories by numerically integrating the equations

$$dx_k/dt = u_x^{(k)},\quad dy_k/dt = u_y^{(k)},\quad dz_k/dt = u_z^{(k)}. \tag{7}$$

By virtue of the linearity of the Stokes and Laplace euqations and boundary conditions (3)-(6), we represent the distributions of the microscopic parameters (v, p, T_e) as

$$v = \sum_{k=1}^{N} v^{(k)},\ p = \sum_{k=1}^{N} p^{(k)},\ T_e = T_{e0} + (\nabla T_e)_\infty r_k + \sum_{k=1}^{N} T_e^{(k)}. \tag{8}$$

Here, $v^{(k)}$, $p^{(k)}$, $T_e^{(k)}$ determine the perturbation of the corresponding field due to the k-th particle. We seek the perturbations $v^{(k)}$, $p^{(k)}$ in the form of the solution of the Lamb equation [6]

$$\begin{aligned} v^{(k)} = \sum_{n=1}^{\infty} \{ & r_0 t_k (r_k \chi_{-n-1}^{(k)}) - (n-2)/(2\eta_e n(2n-1)) \cdot r_k^2 \nabla_k p_{-n-1}^{k} - \\ & - \nabla_k \Phi_{-n-1}^{(k)} + (n+1)/(\eta_e n(2n-1)) \cdot r_k p_{-n-1}^{(k)} \}, \quad p = \sum_{n=1}^{\infty} p_{-n-1}^{(k)}, \end{aligned} \tag{9}$$

while we seek $T_e^{(k)}$ (and T_k) in the form of the general solution of the Laplace equation. In (9), $p_{-n-1}^{(k)}$, $\Phi_{-n-1}^{(k)}$, $\chi_{-n-1}^{(k)}$ are spherical space harmonics of the order $-(n+1)$ and are written in the spherical coordinate system of the k-th particle.

The force acting on the k-th particle is determined from the formula [7]

$$F^{(k)} = -4\pi \nabla_k (r_k^3 p_{-2}^{(k)}). \tag{10}$$

The specific form of the harmonic $p_{-2}^{(k)}$ is found by inserting the distributions of v, T_e, and T_k into (3)-(6). Here, after we satisfy the boundary conditions on the surface of the k-th particle, we must write the perturbations due to the remaining particles in the coordinate system of this particle. These transformations can be performed by means of well-known formulas [8] for systems consisting of just two particles.

In the general case (N > 2), the specific expression for $F^{(k)}$ can be obtained on the basis of the present approach in the so-called two-particle approximation. Here, for a given particle, we consider its hydrodynamic interaction with each remaining particle separately. In this case, it can be shown that only terms of the order $h_{\alpha k}^{n}$ (where n = 0, 1, ..., 5) should be left in expansions of the macroparameters in the small parameter $h_{\alpha k}$. This circumstance also explains why we are not considering particle rotation in the present study. As was shown in the example of systems of two particles [2], the allowance can be made for particle rotation if the calculations are carried out to within terms of the order $h_{\alpha k}^{7}$, inclusively.

Proceeding on the basis of the procedures described above, to within terms of the order $h_{\alpha k}^{5}$, inclusively, we obtain specific expressions for the instantaneous velocities of each of N particles:

$$\begin{aligned} u_z^{(\alpha)} = u_0^{(\alpha)} & \left\{ 1 + \frac{\varkappa_e (1 + 2c_q \mathrm{Kn}^{(k)}) - \varkappa_k (1 - K_T \mathrm{Kn}^{(k)})}{2\varkappa_e (1 - c_q \mathrm{Kn}^{(k)}) + \varkappa_k (1 + 2K_T \mathrm{Kn}^{(k)})} \times \right. \\ & \left. \times \left(1 - 3\cos^2\alpha \left(\frac{R_k}{l_{\alpha k}} \right)^3 \right) \right\} - \frac{1}{2} u_0^{(\alpha)} \frac{2\varkappa_e + \varkappa_k}{2\varkappa_e + \varkappa_\alpha} H^{(k)} \left(\frac{R_k}{l_{\alpha k}} \right)^3 (1 - 3\cos^2\alpha), \\ u_x^{(\alpha)} = & \frac{3}{4} u_0^{(k)} H^k \sin 2\alpha \left(\frac{R_k}{l_{\alpha k}} \right)^3 \frac{2\varkappa_e + \varkappa_k}{2\varkappa_e + \varkappa_\alpha} - \\ - \frac{3}{2} u_0^{(\alpha)} & \frac{\varkappa_e (1 + 2c_q \mathrm{Kn}^{(k)}) - \varkappa_k (1 - K_T \mathrm{Kn}^{(k)})}{2\varkappa_e (1 - c_q \mathrm{Kn}^{(k)}) + \varkappa_k (1 + 2K_T \mathrm{Kn}^{(k)})} \sin 2\alpha (R_k/l_{\alpha k})^3, \ u_y^{(\alpha)} = 0. \end{aligned} \tag{11}$$

Here, $v_0^{(\alpha)}$ is the thermophoretic velocity of a single moderately coarse solid particle;

$$H^{(\alpha)} = \frac{\left[1 + (\beta_b + \beta_R') \mathrm{Kn}^{(\alpha)} + 2 \frac{c_V}{K_{TS}^{(0)}} \mathrm{Kn}^{(\alpha)} \right] \left(1 + \frac{\varkappa_\alpha}{\varkappa_e} K_T \mathrm{Kn}^{(\alpha)} \right) +}{\left[1 + (\beta_b + \beta_R') \mathrm{Kn}^{(\alpha)} - (1 + Gc_m \mathrm{Kn}^{(\alpha)}) \frac{c_V}{K_{TS}^{(0)}} \mathrm{Kn}^{(\alpha)} \right] \left(1 + \frac{\varkappa_\alpha}{\varkappa_e} K_T \mathrm{Kn}^{(\alpha)} \right) +} \rightarrow$$

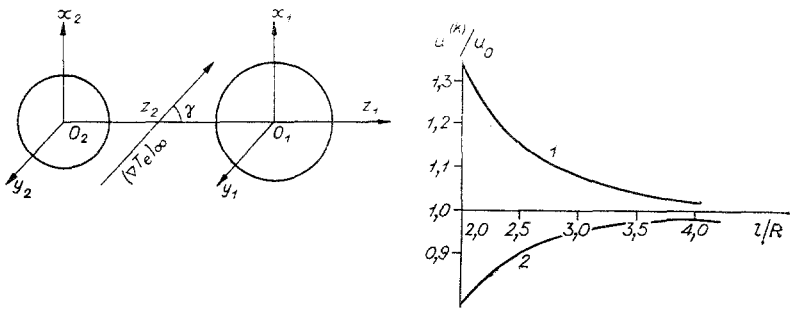

Fig. 1

$$\rightarrow \frac{+(\beta_R-\beta_b)\,\mathrm{Kn}^{(\alpha)}\left(\frac{\varkappa_\alpha}{\varkappa_e}-2c_q\,\mathrm{Kn}^{(\alpha)}\right)}{+(\beta_R-\beta_b)\,\mathrm{Kn}^{(\alpha)}\left(\frac{\varkappa_\alpha}{\varkappa_e}-2c_q\,\mathrm{Kn}^{(\alpha)}\right)}.$$

Equations (11) are written in a laboratory coordinate system in which the Oz axis is directed along the line of centers of particles with the numbers α and k at the angle φ to the vector $(\nabla T_e)_\infty$, while the coordinate plane Oxz is directed parallel to it.

Using (11) and numerically integrating Eqs. (7), we studied the behavior of an ensemble of 30 moderately coarse aerosol particles located either along a straight line (linear ensemble) or on one surface (plane ensemble). In order to numerically solve system (7) on a BÉSM-6 computer, we used the standard application package STIFF [9] to integrate the systems of differential equations. Use of this package makes it possible to solve both stiff and nonstiff problems. The implicit Adams method, with a variable (to 12-20) order, can be used to solve nonstiff problems. Since STIFF is a one-step subroutine, a driver and an executive were written to control it. Having reduced computing time by one order allowed us to replace the Jacobian used to calculate the corrector in the Newton integration process by a unit matrix for particles of the same radii and by a diagonal matrix for particles of different radii. The computation was carried out with an accuracy of 10^{-4} up to the moment of time $\tau = t/n \simeq 2500$ ($\tau = R/u_0$, the choice of τ being dictated by the condition $\tau(R/\ell)^6 \leq 0.1$).

The given program considers the possibility of there being a reduction in the total number of particles in the ensemble as a result of the coalescence (or coarsening) of particles. Two particles with the numbers α and k which approach one another to within a distance on the order of $0.1 \max\{R_\alpha, R_k\}$ are considered to be one particle having the radius $R_{\alpha k} = \sqrt[3]{R_\alpha{}^3 + R_k{}^3}$.

To calculate results for specific points, we resorted to interpolation with the aid of a Taylor series. Without significantly affecting the accuracy of the results, use of the Taylor series allowed us to retain the integration step attained previously in the continuation of calculation. The results of the calculations were output on a graph plotter in the form of a set of lines representing the trajectories of the particles of the ensemble during the time τ. These results are shown in Figs 1-6.

Figures 1-3 show the dependence of the quantity $\delta = u^{(k)}/u_0$ ($u^{(k)}$ is the velocity of a doublet of two identical particles) on the distance between the particles ℓ_{12} (Fig. 1), on the ratio $\varkappa_\alpha/\varkappa_e$ (Fig. 2), and on the Knudsen number Kn (Fig. 3).

Curves 1 pertain to the case when the line of centers of the particles comprising the doublet are parallel to the vector $(\nabla T_e)_\infty$, while curves 2 pertain to the case when the line is perpendicular to the vector.

Figures 4-6 show the results of numerical calculation of the motion of a chain of 30 aerosol particles. It was assumed that the distance between the centers of any two adjacent particles in the chain was initially constant and that the particles were moving at a steady velocity. Figures 4-6 depict the dynamics of chains of identical particles (R_k = 1 μm, k = 1, 2, ..., 30), chains of three kinds of regularly spaced particles ($R^{(1)}$ = 1 μm, $R^{(2)}$ = 3 μm, $R^{(3)}$ = 10 μm), and chains of three kinds of randomly located particles ($R^{(1)}$ = 1 μm,

$R^{(2)}$ = 3 μm, $R^{(3)}$ = 10 μm). All of the results were obtained for κ_α/κ_e = 10 and Kn = 0.3. The particle trajectories in Figs. 4-6 are plotted in a coordinate system connected with the center of mass of the particles. In Figs. 5 and 6, the discontinuity in the trajectory line of each particle corresponds to the coalescence of particles. An analysis of the results permits the following conclusions regarding the behavior of the given systems.

1. In the motion of the particles along the line of centers, an increase in the distance between particles is accompanied by a rapid decrease in hydrodynamic interaction (see Fig. 1). Thus, at ℓ_{12} = 3.086R and κ_k/κ_e = 70, δ = 1.1. When the distance between particles is greater than 10R, the velocity of the doublet is nearly the same as the velocity of single particle. A similar pattern is seen with an increase in Kn (see curve 1 in Fig. 3). With the motion of a doublet along the line of centers, its velocity will be greater than the velocity of a single particle. The additional velocity here may reach 25-30% of the original value. With the motion of the particles perpendicular to the line of centers, δ < 1, i.e., the doublet moves more slowly than a single particle. Here, the dependence of δ on ℓ_{12} and Kn is the same as in the case of the motion of particles along the line of centers (see Figs. 1 and 2, curves 2).

If the line of centers of identical particles makes the angle φ with the direction of $(\nabla T_e)_\infty$, then drift of the doublet takes place, i.e., it moves in the direction perpendicular to $(\nabla T_e)_\infty$. Meanwhile, drift velocity is maximal at φ = π/4.

2. The configuration of a doublet consisting of particles of different radii changes over time. The position of the line of centers will be stable if the smaller particle trails the larger particle (φ = π); the smaller particle moves faster than and overtakes the larger particle (the approach velocity is determined by the parameters $h_{\alpha k}$ and Kn). When the larger particle is moving behind the smaller particle (φ = 0), the position of the line of centers is unstable and small deviations of the line from φ = 0 lead to a further increase in φ and the realization of one of two cases: in the first case φ ≥ π/2, $\ell_{\alpha k} < \ell_{cr}$ (ℓ_{cr} is the value of $\ell_{\alpha k}$ at which particle interaction ceases), the angle φ continues to increase while the distance between particles begins to decrease; in the second case φ < π/2, $\ell_{\alpha k} > \ell_{cr}$, particles continue to move as single particles. It should be noted that here, as in the systems examined in Sec. 1, interaction between the particles decreases with an increase in the number Kn.

3. For a unidimensional ensemble of identical moderately coarse spherical aerosol particles (a chain) whose line of centers is parallel to the gradient $(\nabla T_e)_\infty$, motion takes place

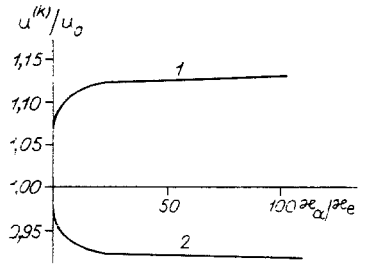

Fig. 2

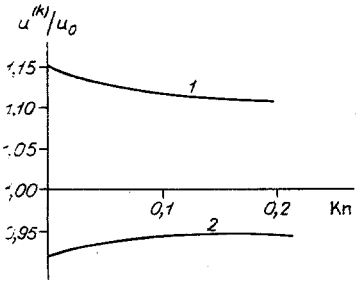

Fig. 3

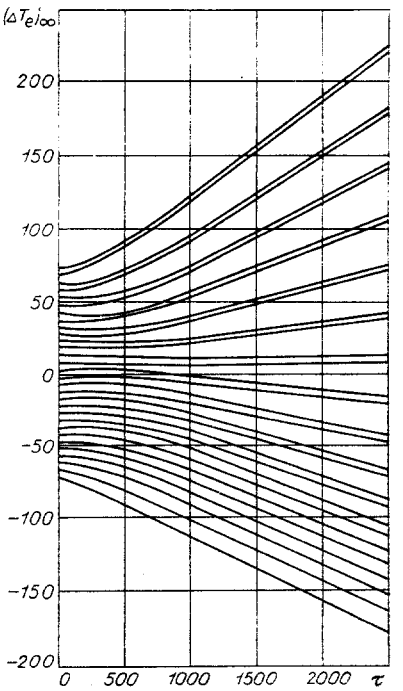

Fig. 4

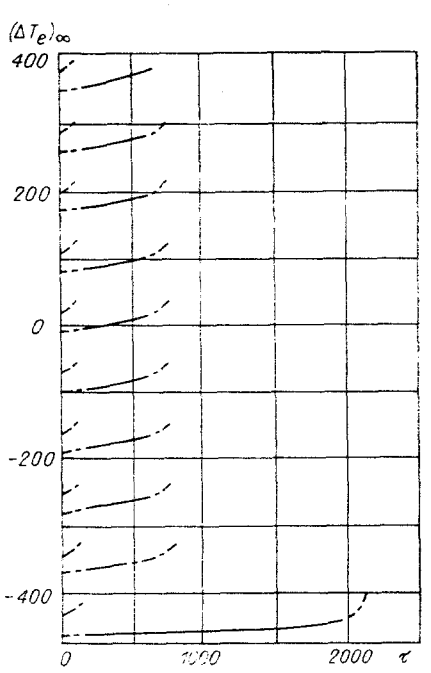

Fig. 5

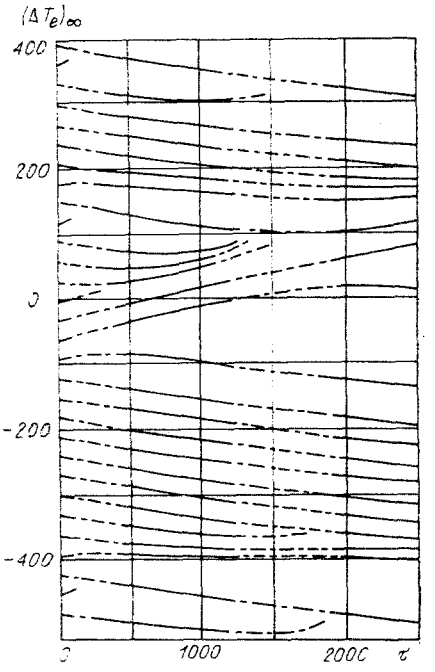

Fig. 6

along the gradient and the ensemble decomposes into isolated doublets and single particles (see Fig. 4). The shortest distance between particle surfaces (the smallest gap) is established in the leading doublet. Thus, the velocity of this doublet is maximal. For the other doublets, the size of the gap is greater, the farther the doublets are from the leading part of the chain, and their thermophoretic velocities decrease in the order corresponding to their location in the chain. The time over which the chain decomposes into isolated doublets and single particles, which undergo almost no interaction, is on the order of minutes for the given system of 30 particles, with R = 1 μm, $\ell_0 = 5R$, and Kn = 0.03. Here, the size of the system (the distance between the outermost particles at the initial moment of the doublets at the final moment) increases threefold.

4. If the ensembles examined in Sec. 3 consist of particles of different radii, then their behavior will differ significantly from the behavior of a chain of identical particles. Two situations can be realized in this case. In the first situation, particles of different radii form a regular system with a regularly repeating sequence of particles (see Fig. 5). In the second situation, particles of different radii are positioned at random in the chain (see Fig. 6). As an example of a linear regular system, we will examine a chain composed of three kinds of particles: R_1 = 10 μm, R_2 = 3 μm, R_3 = 1 μm. Such a system can be schematically represented in the form $R_1R_2R_3R_1R_2R_3 \ldots R_1R_2R_3$. Meanwhile, at the initial moment $\ell_{k,k+1} = \ell_0 = 3R_1$, while $\kappa_k/\kappa_e = 10$. The direction of $(\nabla T_e)_\infty$ was chosen so that the chain moved in the direction of the outermost particle with the radius R_1. The radius of the numerical calculations showed that coarse particles or aggregates are formed in such a system over time (one particle is formed from three successively positioned particles with the radii R_1, R_2, R_3). The process of aggregate formation is completed by the moment of time τ_{cr} = 1 min. Beginning with this moment, the system behaves as a chain consisting of particles of identical radii. It should be noted that the size of the system remains nearly constant in the given case. This happens because particles with the radius R_1 are initially located the distance $12R_1$ apart, i.e., hydrodynamic interaction due to particles of this size has the greatest effect on the motion of adjacent particles in the system we are examining.

In the case of an arbitrary distribution of particles with radii R_1, R_2, R_3 in the chain (see Fig. 6), the behavior of the latter is considerably more complex. In the final analysis, the formation of aggregates causes the initial system to break down into several subsystems – each of which is characterized by a tendency toward further particle coarsening. The number of subsystems and the number of particles in them at a certain fixed moment of time for the systems examined here depend on the initial location of particles in the chain.

The results obtained here – particularly those concerning the possibility of the formation of particle aggregates in a nonisothermal aerosol – may prove useful in performing specific calculations related to the dynamics of such systems. The results might also be used in the design and development of devices for removing aerosol particles from air.

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THERMOCAPILLARY CONVECTION WITH TEMPERATURE-DEPENDENT HEAT RELEASE AT AN INTERFACE

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UDC 536.25

It is known that thermocapillary instability in a system with an interface can be either monotonic or oscillatory in character [1-4]. The stability of the equilibrium state of the system is significantly influenced by presence of heat sources and sinks on the interface due to chemical reaction, evaporation, absorption of radiation, etc. The study [5] solved the problem of stability of equilibrium in a two-layer system against mononotonic perturbations under conditions of surface heat release. Nepomnyashchii and Simanovskii [6] examined the stability of a two-layer system against monotonic and oscillatory perturbations in the presence of temperature-independent heat release at the interface.

In the present investigation, we solve the same problem with allowance for the temperature dependence of surface heat release. It is shown that in certain cases this dependence can lead to expansion of the region associated with oscillatory instability.

1. Let the space between two solid horizontal plates $y = a_1$ and $y = -a_2$, kept at constant temperatures T_1 and T_2, be filled by two layers of viscous immiscible fluids. The x-axis is directed horizontally, while the y axis is directed vertically upward. We assume that thermocapillary convection occurs in the presence of gravity, which in turn allows us to consider the interface to be planar and nondeformable ($y = 0$). Despite this, the effect of buoyancy on convection is assumed to be negligible compared to the thermocapillary effect – as is seen for thin films of liquid. The absolute and kinematic viscosities, thermal conductivities, and diffusivities are equal to η_m, ν_m, κ_m, χ_m ($m = 1$ for the top fluid and $m = 2$ for the bottom fluid). Surface tension is linearly dependent on temperature: $\sigma = \sigma_0 - \alpha T$.

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