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Mathematical modeling of dispersed media flows in the presence of nucleation, coagulation and phase transitions

A model of motion of a gas-dispersed medium in the presence of processes of nucleation, coagulation and phase transitions has been constructed. A homogeneous nucleation model is used to describe the nucleation process. It is believed that the process of cluster coagulation occurs due to their Brownian motion. The analysis of the solution of the coagulation equation in the particular case of monodisperse clusters in the presence of a source and sink of particles is carried out. To determine the rate of phase transitions the Hertz-Knudsen-Langmuir formula is used. The calculations were carried out on the basis of a quasi-one-dimensional model within the equilibrium approximation (when the velocities and temperatures of the phases coincide). As a result of the study the main properties of the flow of a two-phase mixture in a channel in the presence of nucleation, coagulation, and phase transformations have been established. It is shown that the vapor temperature increases along the channel and reaches the saturation temperature at some distance from the channel entrance. Calculations have shown that the coagulation process has a rather strong effect on the distribution of cluster sizes along the channel.

Keywords: dispersed mixture, nucleation, coagulation, phase transitions, Brownian motion.

Introduction

In practice there are often processes in which in the initial state the working medium is single-phase, for example, in the form of a gas (vapor), and during the process under study conditions are created for the appearance of a new phase in the form of drops (nuclei) [1–3]. It is these processes that determine the initial stage of phase transitions in single-phase (in the initial state) media (for example, in supercooled vapor). Fluctuation, nucleation and further condensation growth of clusters in a supersaturated vapor is one of the most important processes leading to the nucleation and development of a dispersed phase. Note that the problem of mathematical description of the process of nucleation remains relevant to this day. Recently it has been actively discussed in connection with the study of the growth of nanoclusters in dispersed systems [2–5].

The nuclei of the liquid phase that appeared as a result of nucleation are rather small (nanoscale) and therefore are subject to Brownian wandering. Brownian wandering leads to their mutual collision, therefore it is one of the main constantly acting mechanisms that contribute to the coagulation of microdroplets. Coagulation (fusion) of particles is one of the main reasons for the evolution of dispersed systems, which include various mixtures of a medium (gaseous or liquid) with particles (solid or liquid). This phenomenon is observed in various physical situations and affects the growth of clusters in solutions, gas-dispersed systems [6–8].

Evaporation and condensation processes in various media are used to obtain nanomaterials (in particular, in the synthesis of carbon nanotubes), as well as to obtain nano- and ultradispersed particles in expanding channels due to nucleation and their growth [9–13].

Thus, the study of flows of two-phase systems in channels of constant and variable cross-sections in the presence of various processes (nucleation, coagulation of nuclei, phase transitions) is of theoretical and practical interest and is relevant.

In what follows, along with the term “nucleus”, we will also use the terms “cluster” or “particle”.

Homogeneous nucleation kinetics

In the presence of foreign particles (impurities, ions, etc.), vapor condensation mainly occurs on impurity particles (heterogeneous nucleation). In this case it is enough just to create a state of supersaturation. In a pure supersaturated vapor the initial state is metastable and the condensation process begins only when nuclei of the liquid phase (microdroplets or clusters) appear with a size greater than a certain critical value, since supercritical clusters are stable and it is thermodynamically advantageous for them to grow further (homogeneous nucleation) [1, 3]. The molecular kinetic theory of the homogeneous nucleation process was laid down in the works of a number of researchers. This theory is based on the fact that in a gas, as a result of fluctuations in the concentration of molecules in their chaotic motion, clusters are continuously formed and destroyed (microdroplets in supercooled vapor). Further, only spherical clusters will be considered. In the case of a Maxwellian velocity distribution of molecules, the distribution of these clusters on the radius is described by the Gibbs formula

$$N(a) = N_1 \exp\left[-\frac{\delta Z(a)}{k_B T}\right],$$

where N_1 is number of carrier phase molecules per unit volume, k_B is Boltzmann's constant, T is carrier medium temperature, $\delta Z(a)$ is the so-called work of creating a cluster of radius a. The work $\delta Z(a)$ is equal to the change in the Gibbs thermodynamic potential for the substance included in the cluster, taking into account the contribution to create the surface of the liquid phase [1]

$$\delta Z(a) = \frac{4}{3}\pi a^3 \overset{\circ}{\rho}_2 \Delta z + 4\pi a^2 \sigma, \quad \Delta z = z_2(p,T) - z_1(p,T).$$

Here z is Gibbs potential, σ is surface tension, $\overset{\circ}{\rho}_2$ is density of condensed phase. In the metastable state, when $z_2 < z_1$ (supercooled steam or superheated liquid) $\delta Z(a)$ has the maximum at the $a = a_*$

$$a_* = -\frac{2\sigma}{\overset{\circ}{\rho}_2 \Delta z}, \quad \delta Z(a_*) \equiv E_* = \frac{4}{3}\pi a_*^3 \sigma.$$

The value of a_* is called the critical radius of nuclei, and the value E_* is the work of creating a critical nuclei. Thus, if a cluster with a size $a > a_*$ arises in the metastable carrier phase, then it should grow, since this leads to a decrease in the thermodynamic potential of the system. Such a supercritical cluster may turn out to be the nucleus of a new dispersed phase. Subcritical clusters with a radius $a < a_*$ should disappear, since this also leads to a decrease in the thermodynamic potential. Hence, it follows that the emergence of "viable" nuclei is associated with overcoming the potential or activation barrier E_*, so this value serves as a measure of the stability of the metastable state of the system, as well as a measure of the probability of the fluctuation appearance of a new dispersed phase. Using the linear expansion of the Gibbs potential near the saturation state along the isotherm for supercooled vapor, we obtain [1]:

$$a_* = \frac{2\sigma \bar{\overset{\circ}{\rho}}_{1s}}{(p - p_s)(1 - \bar{\overset{\circ}{\rho}}_{1s})}, \quad E_* = \frac{16\pi}{3}\sigma^3 \left[\frac{\bar{\overset{\circ}{\rho}}_{1s}}{(p - p_s)(1 - \bar{\overset{\circ}{\rho}}_{1s})}\right]^2, \quad \bar{\overset{\circ}{\rho}}_{1s} = \frac{\overset{\circ}{\rho}_{1s}}{\overset{\circ}{\rho}_{2s}}, \tag{1}$$

where $\overset{\circ}{\rho}_{1s}$, $\overset{\circ}{\rho}_{2s}$ are real densities of the gaseous and liquid phases at saturation. The concentration of critical nuclei is determined by the formula

$$N(a_*) \equiv N_* = N_1 \exp\left(-\frac{E_*}{k_B T}\right). \tag{2}$$

One can imagine the following sequence of the dispersed phase clustering process [1, 9]. With an increase in supersaturation the size of critical nuclei decreases and the probability of their occurrence increases. The onset of the phase transition is determined by the probability of the appearance of nuclei of precisely the critical size. The rate of formation of nuclei of critical size is high and, based on (2), amounts to approximately 10^{19} nuclei per unit volume, and therefore, despite their small size ($a_* \sim 10^{-9}$ m), the total surface on which condensation occurs is rather large. Due to the rapid formation of nuclei and their further growth, there is an intense increase in the mass of the liquid phase and the release of heat. Usually the appearance of even a small amount of liquid can significantly affect the flow parameters. The release of heat leads to a decrease in the degree of supersaturation, as a result of which the formation of new nuclei stops, and further clustering occurs already at the newly formed condensation centers. So, all condensation centers arise, as a rule, at the very beginning of the nucleation process, when a sufficiently large supersaturation takes place. After that, the transition from the metastable state to the saturation state can occur rather quickly and be of a discontinuous nature. It follows that the clustering process in high-speed streams can be divided into two stages. At the first stage the decisive factor is the formation of nuclei of a critical size; at the second the process of condensation growth of newly formed nuclei, when nucleation can be ignored. Although in some cases both processes occur simultaneously, such a division seems to be quite reasonable.

Note that the problem of mathematical description of the process of nucleation remains relevant to this day.

The equation of coagulation

Small (nanoscale) particles react to random molecular fluctuations in the density and average velocity of the molecules of the medium, therefore they are constantly in irregular (Brownian) motion. Brownian wandering leads to their mutual collision, therefore it is one of the main constantly acting mechanisms that contribute to the coagulation of small particles. When constructing a mathematical model of the coagulation process, the following physical assumptions are imposed on the dispersed system [7, 8]: the number of particles is large enough to apply the distribution function of the number of particles by mass; the dispersed system is so rarefied that only pair collisions of particles can be considered, and triple and higher-order interactions can be neglected; particles of a dispersed system form a chaotic set. These conditions are necessary for the statistical description of the system and are important for simplifying the mathematical modeling of the process under study. A discrete version of the kinetic equation of coagulation was first formulated in 1916 by the Polish scientist M. Smoluchowski.

Note that sometimes (for example, in the case when liquid drops act as particles) it is convenient to write down the coagulation equation in terms of the volumes of particles, which in the continuous version has the form

$$\frac{dn(\nu,t)}{dt}=\frac{1}{2}\int_0^{\nu}K(\phi,\nu-\phi)n(\phi,t)n(\nu-\phi,t)d\phi-\int_0^{\infty}K(\phi,\nu)n(\phi,t)n(\nu,t)d\phi\,, \qquad (3)$$

where ν, ϕ are the particles volumes, K is coagulation kernel (is symmetric in its arguments), $n(\nu,\ t)$ is number of particles with the volume ν in per unite of volume of mixture. Equation (3) is a nonlinear integro-differential equation. To date, a significant number of approximate and numerical methods for solving the kinetic equation of pair coagulation have been developed. However, a closed analytical solution can be obtained only for model kernels [6-8].

To determine the total number of particles per unit volume, it is necessary to integrate the value of $n(\nu,t)$ over all volumes of particles

$$N(t)=\int_0^{\infty}n(\nu,t)d\nu\,.$$

Then the change in the total number of particles over time will be equal to

$$\frac{dN(t)}{dt}=-\frac{1}{2}\int_0^{\infty}\int_0^{\infty}K(\nu,\phi)n(\nu,t)n(\phi,t)d\nu d\phi\,. \qquad (4)$$

If spherical clusters coagulate by the collisions due to Brownian motion, then the kernel of the kinetic coagulation equation (3) has the form [5]

$$K(\nu_1,\nu_2)=4\pi(D_1+D_2)(a_1+a_2)\,,$$

where a_1, a_2, ν_1, ν_2, D_1, D_2 are radii, volumes and diffusion coefficients of particles. In the case of coagulation of monodisperse spherical particles (when $D_1=D_2=D$, $a_1=a_2=a$) the coagulation core will take on a simple form $K=16\pi Da$. The particle diffusion coefficient is determined from the theory of Brownian motion developed by Einstein [5]. According to this theory

$$D=\frac{k_BT}{6\pi\mu a}\,,$$

where μ is viscosity of carrier medium. Thus, the coagulation kernel in the case of monodisperse spherical particles subject to Brownian wandering will finally be written in the form

$$K=K_0=\frac{8}{3}\frac{k_BT}{\mu}\,.$$

In this case, the equation for the total number of particles in the dispersed system (4) takes the simpler form

$$\frac{dN}{dt} = -\frac{K_0}{2} N^2 . \tag{5}$$

If the sizes of the clusters are very small and close to the mean free path of the molecules of the medium, the force of resistance to the motion of the particle should be less than that predicted by Stokes' law. This effect is usually taken into account using the Cunningham-Millikan correction [5]. Then for the coagulation kernel we have

$$K_0 = \frac{8}{3}\frac{k_B T}{\mu} C_M , \qquad C_M = 1 + \frac{\lambda}{a}\left[A + Q \exp\left(-\frac{ba}{\lambda} \right) \right] .$$

If there is a constant or variable source of particles in a dispersed system (for example, due to the process of nucleation or condensation) or a sink of particles (for example, due to evaporation, deposition of particles on various surfaces or gravitational sedimentation), then equation (5) is modified and written in form

$$\frac{dN}{dt} = \psi - \frac{K_0}{2} N^2 , \tag{6}$$

where ψ is the rate of appearance ($\psi>0$) or disappearance ($\psi<0$) of particles per unit volume of the mixture. Since the coalescence of particles (liquid droplets) does not change the total volume of the dispersed phase, the change in the volume of the dispersed phase in the system is caused only by the appearance of new particles due to the source or their disappearance from the system in the presence of a drain. For simplicity, let us assume that particles that reappear due to a source or disappear due to a sink are of the same size as the coagulating particles (this assumption is valid, at least in the case of particle sink or at the beginning of the coagulation process in the presence of a source). Then, for the volumetric content of the dispersed phase α_2, the following equation can be written

$$\frac{d\alpha_2}{dt} = \frac{4}{3}\pi a^3 \psi , \qquad \alpha_2 = \frac{4}{3}\pi a^3 N .$$

Hence, taking into account Eq. (6), we obtain an equation for the rate of change in the radius of particles

$$\frac{da}{dt} = \frac{K_0}{6} aN . \tag{7}$$

From (6) it follows that at a constant positive value of ψ, the concentration of particles tends to an equilibrium value with time $N_\infty = \sqrt{2\psi / K_0}$, and this equilibrium state is stable, since

$$\frac{\partial F}{\partial N} < 0 , \quad F = \psi - \frac{K_0}{2} N^2 .$$

In the simple case K_0=const, the Eq. (6) has an exact solution, which can be written in dimensionless variables as

$$\overline{N} = \frac{A\exp(\omega t) - 1}{A\exp(\omega t) + 1}, \quad \overline{N} = \frac{N}{N_\infty}, \quad N_\infty = \sqrt{\frac{2\psi}{K_0}}, \quad A = \frac{1+\overline{N}_0}{1-\overline{N}_0}, \quad \omega = \sqrt{2\psi K_0} , \tag{8}$$

where $\overline{N}_0$ is dimensionless initial concentration of particles. From (8) it follows that the concentration of particles reaches its limiting value $\overline{N}$ =1 over infinite time. Taking into account the expression (8), Eq. (7) has the following solution, which shows the law of variation of the radius of coagulating particles

$$\overline{a} = \left[\frac{A\exp(\omega t) + 1}{(A+1)\exp(\omega t / 2)} \right]^{1/3}, \quad \overline{a} = \frac{a}{a_0} . \tag{9}$$

Here a_0 is initial radius of particles. At the large time, when ωt>>1 the particle radius changes according to the law

$$\overline{a} \cong \left(\frac{A}{A+1} \right)^{1/3} \exp(\omega t / 6) .$$

At a constant negative value $\psi<0$ the equilibrium state for a dispersed system does not exist and the concentration of particles tends to zero with time. In this case, the equation for the concentration of particles takes the form

$$\frac{dN}{dt} = -\varphi - \frac{K_0}{2} N^2 , \quad (\varphi=-\psi, \ \ \varphi>0).$$

The solution of this equation is the function

$$\overline{N}=\frac{1-B\tan(\omega t/2)}{1+\frac{1}{B}\tan(\omega t/2)},\quad \overline{N}=\frac{N}{N_0},\quad B=\frac{1}{N_0}\sqrt{\frac{2\varphi}{K_0}},\quad \omega=\sqrt{2\varphi K_0}\,. \tag{10}$$

Hence it follows that the concentration of particles reaches zero in a finite time $t_*=(2/\omega)\arctan(1/B)$. Moreover, with increasing parameter *B*, the time of disappearance of the dispersed phase in the system decreases and tends to the limiting value $t_*=\pi/\omega$. This means that the presence of a sink, even of infinitely low intensity, will lead to the disappearance of particles (a drop in the concentration of particles to zero) in a finite time. In the presence of a dispersed phase drain for the particle radius we have the following formula

$$\overline{a}=\left\{\frac{\left[1+(1/B)\tan(\omega t/2)\right]^2}{1+\left[\tan(\omega t/2)\right]^2}\right\}^{1/6}. \tag{11}$$

The limiting particle radius corresponding to the instant of disappearance $t=t_*$ can be calculated by the formula

$$\overline{a}(t_*)=\left(1+\frac{1}{B^2}\right)^{1/6}.$$

From the last formula it follows that with an increase in the parameter *B* the limiting radius of particles decreases. Figure 1 below shows the approximate behavior of solutions (8) and (9) corresponding to the presence of a source of new particles in the mixture for various values of the initial concentration of particles $\overline{N}_0$=0 (curve *1*), 0.5 (*2*), 2 (*3*), 5 (*4*). Note that although the concentration of particles tends to a finite limiting value over time, the size of the clusters increases theoretically indefinitely. Figure 2 illustrates the behavior of solutions (10) and (11) corresponding to the presence of a particle sink in the dispersed system. Curves *1–6* correspond to the values of the parameter *B*=0.01, 0.05, 0.1, 0.25, 0.5, 1, respectively. In Figure 2*b* the points where the curves end correspond to zero particle concentration.

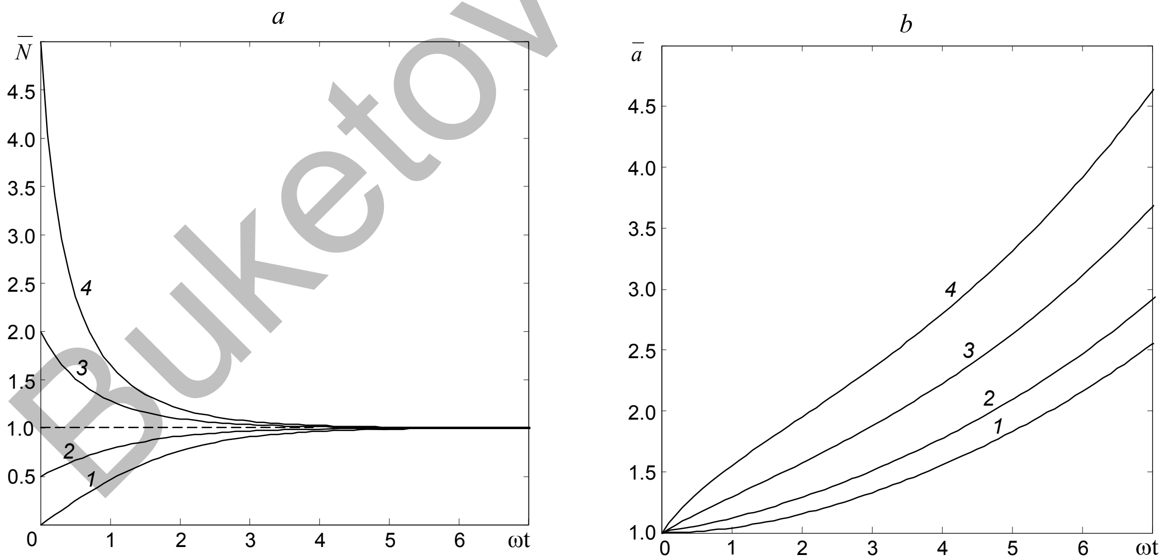

Figure 1. The graphs of dependency (8) (*a*) and (9) (*b*): curves *1* - $\overline{N}_0$=0; *2* - 0.5, *3* - 2, *4* - 5

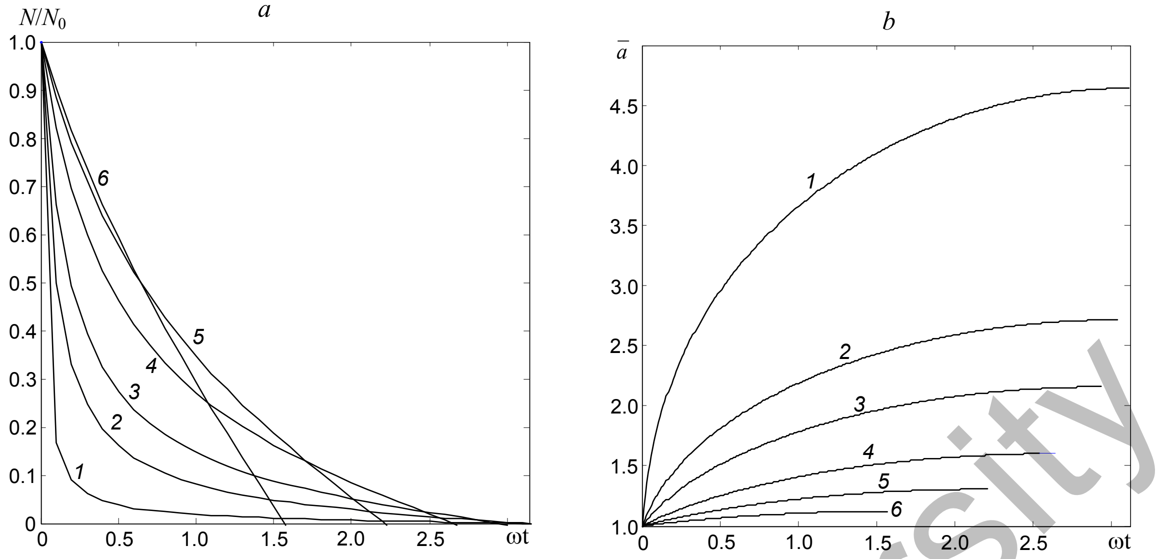

Figure 2. The behavior of the solution (10) (*a*) and (11) (*b*): curves *1* - *B*=0.01; *2* - 0.05; *3* - 0.1; *4* - 0.25; *5* - 0.5; *6* - 1

Kinetics of phase transitions

Analysis of the processes of entrainment and deposition of vapor molecules at the interface leads to the Hertz-Knudsen-Langmuir formula for the resulting intensity of phase transitions [1]

$$\xi_{12} = \frac{\beta_m}{\sqrt{2\pi R_g T_s}}(p - p_s), \tag{12}$$

where p is pressure in gas, p_s, T_s are the saturation pressure and temperature, R_g is gaseous constant, β_m is accommodation coefficient, showing the fraction of adsorbed vapor molecules falling on the surface of the liquid (the remaining fraction $1-\beta_m$ is specularly reflected from the surface). The accommodation coefficient depends on the contacting phases and varies in a wide range (from very small values to values close to unity). In formula (12) the saturation temperature corresponds to a given vapor pressure $T_s = T_s(p)$.

The dependence of the phase saturation temperature on pressure satisfies the Clapeyron-Clausius differential equation [1]:

$$\frac{dT_s}{dp} = \frac{T_s}{l}\left(\frac{1}{\rho_{1s}^{\circ}} - \frac{1}{\rho_{2s}^{\circ}}\right). \tag{13}$$

Here $l(p)$ is heat of vaporization. Taking into account the Clapeyron-Clausius equation, the intensity of the phase transition determined by formula (12) can be expressed in terms of superheating (for evaporation) or supercooling (for condensation)

$$\xi_{12} = K_\beta \frac{T_s - T}{T_s}, \qquad K_\beta = \frac{\beta_m l \rho_1^{\circ}}{\sqrt{2\pi R_g T_s}}. \tag{14}$$

The equations for dispersed mixture flows

Thus, taking into account the assumptions and equations given in the introduction and previous sections, the following system of equations can be written to describe the flow of a dispersed mixture in the quasi-one-dimensional stationary case in the presence of processes of nucleation, coagulation of nuclei, and phase transitions:

$$\frac{dm_1}{dx} = -J_{12}, \quad \frac{dm_2}{dx} = J_{12}, \quad \frac{dnvS}{dx} = -\frac{K_0}{2}n^2 S, \tag{15}$$

$$m\frac{dv}{dx} = -S\frac{dp}{dx}, \quad m_1\frac{di_1}{dx} = \alpha_1 vS\frac{dp}{dx} - J_{12}(i_2 - i_1), \quad m_2\frac{di_2}{dx} = \alpha_2 vS\frac{dp}{dx}, \tag{16}$$

$$m = m_1 + m_2, \quad m_k = \rho_k v_k S, \quad \rho_k = \rho_k^{\circ}\alpha_k, \; k = 1,2, \quad \alpha_1 + \alpha_2 = 1, \quad \alpha_2 = \frac{4}{3}\pi a^3 n, \quad K_0 = \frac{8k_B T}{3\mu_1}.$$

Here the subscripts 1 and 2 refer to the parameters of the gaseous and condensed phases, respectively; $\rho^\circ, \rho, \alpha, i$ are real and reduced density, volumetric content and phase enthalpy; p, v, n are pressure in the gas, velocity of mixture, concentration of nuclei; x, $S(x)$ are longitudinal coordinate and cross-sectional area of the channel; J_{12} is the intensity of the phase transition, K_0 is the coagulation coefficient of the droplets. Note that due to the small size of the nuclei, the velocities and temperatures of the carrier and condensed phases can be assumed to coincide with each other ($v_1=v_2=v$, $T_1=T_2=T$).

To close the system (15), (16) it is necessary to specify the thermodynamic equations of state of the phases. Here the gas will be considered calorically perfect with constant heat capacity, and the substance of the condensed phase – incompressible. Then we will have [1, 14–15]:

$$\overline{N} = \frac{1 - B\tan(\omega t/2)}{1 + \frac{1}{B}\tan(\omega t/2)}, \quad \overline{N} = \frac{N}{N_0}, \quad B = \frac{1}{N_0}\sqrt{\frac{2\varphi}{K_0}}, \quad \omega = \sqrt{2\varphi K_0}\,. \tag{10}$$

$$p = \rho_1^\circ RT\,, \quad i_1 = i_{10} + c_1(T - T_0), \quad i_2 = i_{20} + c_2(T - T_0) + (p - p_0)/\rho_2^\circ, \tag{17}$$

$$(\rho_2^\circ, c_1, c_2, R = const\ ),$$

where c_1, c_2 are heat capacities of gaseous and dispersed phases; R is gaseous constant; i_{10}, i_{20}, T_0, p_0 are parameters of the medium in some fixed (for example, initial) state, relative to which all changes are counted. It should be borne in mind that the enthalpy of vapor in the general case depends on the pressure and is related to the enthalpy of the liquid phase. In cases where the pressure and temperature are changing in not very wide ranges, and the pressures themselves are not very high one can get by with the model of a calorically perfect gas (17). In this case the necessary condition of suitability (17) is provided if the dependence for the heat of vaporization is described by the following formula [1]:

$$l(p) = l(p_0) - (c_2 - c_1)(T_s(p) - T_s(p_0)) - (p - p_0)/\rho_2^\circ\,. \tag{18}$$

For the saturation temperature $T_s\,(p)$ of the phases we have the Clapeyron-Clausius equation (13).

The phase transition intensity is defined as

$$J_{12} = 4\pi a^2 n \xi_{12} S\,, \tag{19}$$

where ξ_{12} is rate of the phase transition per unit area of the interphase surface, which is determined by the formula (14).

To formulate the problem let us set the following initial conditions at the entrance to the channel:

$$\overline{N} = \frac{1 - B\tan(\omega t/2)}{1 + \frac{1}{B}\tan(\omega t/2)}, \quad \overline{N} = \frac{N}{N_0}, \quad B = \frac{1}{N_0}\sqrt{\frac{2\varphi}{K_0}}, \quad \omega = \sqrt{2\varphi K_0}\,. \tag{10}$$

$$x=0, \quad a = a_*\,, \quad n = N_*\,, \quad p = p_0\,, \quad T = T_0 < T_{s0}\,, \quad v = v_0\,, \quad S = S_0\,, \quad (T_s = T_s(p_0) \equiv T_{s0}). \tag{20}$$

Here a_*, N_* are critical radius and concentration of nuclei corresponding to the initial vapor supersaturation at the channel inlet and calculated by formulas (1) and (2).

The system of equations (15), (16) with closing relations (13), (17–19) and initial conditions (20) represents the Cauchy problem for calculating the mixture flow in a channel of variable cross-section in the presence of nucleation processes, coagulation of nuclei (clusters) and phase transitions. This system has the following first integrals

$$m_1 + m_2 = const\,, \qquad m_1\left(i_1 + \frac{v^2}{2}\right) + m_2\left(i_2 + \frac{v^2}{2}\right) = const\,, \tag{21}$$

reflecting the laws of conservation of mass and energy of a dispersed mixture. They can be used to check the results of numerical integration of system (15), (16).

Thus, the constructed mathematical model makes it possible to calculate the flow of a condensing medium in the presence of processes of nucleation, coagulation of nuclei, and phase transitions in the quasi-one-dimensional approximation.

The calculation results and their analysis

It is not possible to find an analytical solution of the problem formulated above. Therefore, below we analyze some of the calculation results obtained by numerical integration of the system by the Runge-Kutta method of the fourth order of accuracy. The first integrals (21) were used to control the accuracy of the obtained solutions. The calculations were carried out for water vapor and water droplet nuclei. The initial values of the governing parameters at the channel inlet are as follows: pressure p_0=1 MPa, saturation temperature corresponding to this pressure [16] T_{s0}=453 K, vapor supercooling degree is $\theta=(T_{s0}-T_0)/T_{s0}=0.044$. The critical nucleus radius and critical number of clusters calculated by formula (1), (2) are equal to a_*=0.6 nm, $N_*=10^{19}$. For convenience, the velocity of the medium is related to the initial speed of sound in the gas at the inlet and the other parameters are related to the corresponding values at the channel inlet.

Figure 3*a* shows the behavior of the mixture parameters along the channel in the absence of coagulation and channel expansion, but in the presence of nucleation and phase transitions. It can be seen that the presence of phase transitions at the interface (on the surface of nuclei) leads to a decrease in the velocity of the dispersed mixture, an increase in pressure, gas and dispersed phase densities, and the concentration of clusters. It should be noted that the change in the parameters of the mixture occurs in the initial section (~0.02 m long) and then, after reaching the saturation state, the parameters of the disperse system do not change.

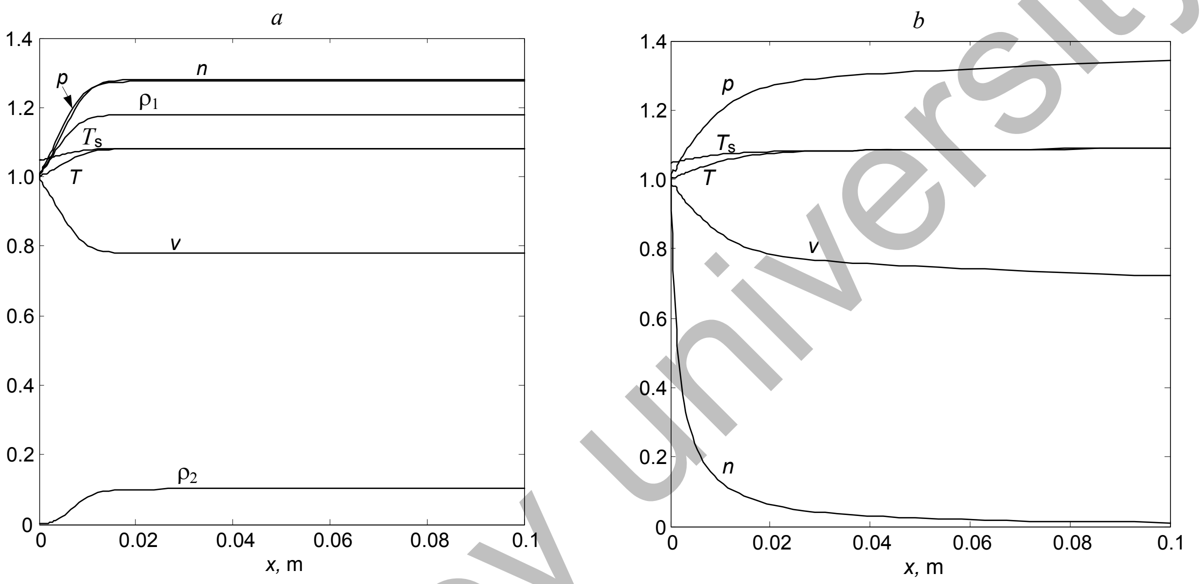

Figure 3. Behavior of the mixture parameters along the channel: *a* – no coagulation and channel expansion; *b* – the presence of coagulation of nuclei and expansion of the channel

The influence of the process of nuclei coagulation and the effect of channel expansion is illustrated in Figure 3*b*. As an example, the flow of a gas-dispersed mixture in a channel in the form of a paraboloid of revolution is considered. In this case for the channel cross-sectional area we have $\overline{S}(x)=S/S_0=1+\kappa x$, where the coefficient κ characterizes the degree of expansion (κ>0) of the channel cross-section per unit length (has a dimension of 1/m). For Figure 3*b* the expansion coefficient is κ=0.5. It can be seen that in spite of the deceleration of the medium along the channel the concentration of nuclei rather strongly decreases along the channel length due to the presence of coagulation. The pressure and temperature of the medium, as in the previous case, increase along the channel and the velocity decreases.

Figure 4 shows the change in the radius of clusters due to the processes of coagulation and phase transitions (condensation). Curves *1* and *2* correspond to different values of the accommodation coefficient β_m=0.001 and 0.01 in the presence of phase transition (condensation) and coagulation processes in a channel without expansion (κ=0), curve *3* shows the change in the radius of nuclei in an expanding channel with an expansion coefficient (κ=0.5) at β_m=0.001, and curve *4* corresponds to the absence of coagulation. In the absence of coagulation the nucleus radius changes only due to the phase transition (curve *4*). Moreover, first there is vapor condensation, then there is an insignificant evaporation of drops, so that the direction of the phase transition changes along the channel. Figure 4 shows that in this case the cluster radius increases by about 8 times. In the presence of the coagulation process the nucleus radius along the channel increases significantly (for example, at a distance of 0.1 m from the channel entrance the nucleus radius increases by about 40 times). Thus, the coagulation process significantly affects the growth of clusters during the flow of a mixture of vapor and nuclei of the condensed phase in the channel. A change in the accommodation coefficient has a rather noticeable effect on the growth of nuclei in the carrier medium, mainly in the initial section of the channel (curves *1* and *2*).

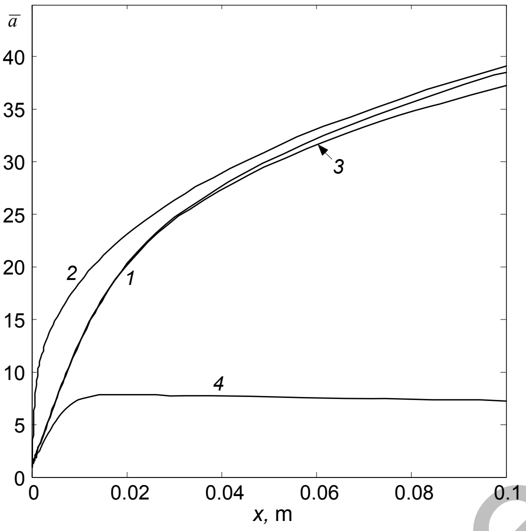

Figure 4. Changing the radius of clusters (the curves are explained in the text).

Conclusion

On the basis of the constructed model of the flow of a dispersed mixture, which takes into account the presence of nucleation, coagulation, and phase transitions, the calculations of the flow of a vapor-droplet mixture in channels of constant and variable cross sections have been carried out. The basic properties of the behavior of the parameters of the mixture along the channel are established. In particular, it was found that the pressure and temperature of the medium increase along the channel, while the velocity decreases. Moreover, the process of cluster coagulation leads to a significant increase in the particle size. Particular solutions of the coagulation equation in the presence of sources and sinks of monodisperse clusters are considered separately.

The results obtained can be useful in various areas of modern technology: in the design of various heat and power and heat exchange plants, to study the process of the outflow of various mixtures from containers, to simulate the processes of formation and growth of nuclei (in particular, nanoclusters) in saturated media, etc.

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Т.Р. Аманбаев, Ғ.Е. Тілеуов, А. Зұпарбекова

Нуклеация, коагуляция және фазалық өзгерістер жағдайындағы дисперсті орталардың қозғалысын математикалық кескіндеу

Нуклеация, коагуляция және фазалық ауысулар болған кезде газдисперсті ортаның қозғалыс моделі құрылады. Кластерлердің пайда болу процесін сипаттау үшін гомогенді нуклеация моделі қолданылды. Кластерлердің коагуляция процесі олардың броундық қозғалысының есебінен жүреді деп саналады. Монодисперсті кластерлердің нақты жағдайында коагуляция теңдеуінің шешімін бөлшектердің пайда болу көзі мен олардың жоғалу үдерістерінің қатысуымен талдау жасалған. Фазалық ауысулардың жылдамдығын анықтау үшін Герц-Кнудсен-Ленгмюр формуласы пайдаланылған. Есептеулер тепе-теңдік шегінде (фазалардың жылдамдықтары мен температуралары сәйкес келген кезде) квазиөлшемді модель негізінде жүргізілді. Зерттеу нәтижесінде каналдағы екі фазалы қоспа ағынының нуклеация, коагуляция және фазалық түрленулер болған кездегі негізгі қасиеттері анықталды. Бу температурасы канал бойымен өсіп, қанығу температурасына канал кіреберісінен біраз қашықтықта жететіндігі көрсетілген. Есептеулер көрсеткендей, коагуляция процесі канал бойымен кластер өлшемдерінің таралымына қатты әсер етеді.

Кілт сөздер: дисперсті қоспа, нуклеация, коагуляция, фазалық түрлену, броундық қозғалыс.

Т.Р. Аманбаев, Г.Е. Тилеуов, А. Зупарбекова

Математическое моделирование течений дисперсных сред при наличии нуклеации, коагуляции и фазовых переходов

Построена модель движения газодисперсной среды при наличии процессов нуклеации, коагуляции и фазовых переходов. Для описания процесса зародышеобразования использована модель гомогенной нуклеации. Считается, что процесс коагуляции кластеров происходит за счет их броуновского движения. Проведен анализ решения уравнения коагуляции в частном случае монодисперсных кластеров при наличии источника и стока частиц. Для определения скорости фазовых переходов применена формула Герца-Кнудсена-Ленгмюра. Расчеты проведены на основе квазиодномерной модели в рамках равновесного приближения (когда скорости и температуры фаз совпадают). В результате исследования установлены основные свойства течения двухфазной смеси в канале при наличии нуклеации, коагуляции и фазовых превращений. Показано, что температура пара увеличивается вдоль канала и достигает температуры насыщения на некотором расстоянии от входа в канал. Расчетами доказано, что процесс коагуляции достаточно сильно влияет на распределение размеров кластеров вдоль канала.

Ключевые слова: дисперсная смесь, нуклеация, коагуляция, фазовые переходы, броуновское движение.

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