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About use of a method of direct numerical solution for simulation of bulk condensation of supersaturated vapor

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ABSTRACT

The results of direct numerical solution of the kinetic equation for the droplet size distribution function are presented. This method which is not restricted by the Knudsen number was developed using the analogy with a similar method of solution of the Boltzmann kinetic equation. The simulation of vapor behavior at fast creation of supersaturation state in vapor–gas mixture by means of adiabatic expansion was carried out for the verification of the method. The results obtained by this method were compared with those which were obtained by using the method of moments over a broad range of Knudsen number. The relevance of taking into account the dependence between saturation pressure and droplet size on the dynamics of condensational relaxation was studied.

1. Introduction

Description of bulk condensation kinetics in various devices includes numerical solution of system of equations for condensation kinetics and gas dynamics in formulation which corresponds to solved problem. Apparently, this approach was proposed in [1]. Results of such solution have concrete character, and in general they can be applied only to a considered case. Alternative idea, which was proposed and implemented in [2–4], is choose of such method of treatment for obtained calculation data in order for results for simple problem to have general character. In the mentioned papers a simulation of vapor behavior in a mixture with non-condensing gas at adiabatic expansion was such simple problem (statement of a problem is submitted below).

Simulation of bulk condensation of supersaturated vapor was carried out on the basis of the numerical solution of the kinetic equation for droplet size distribution function by method of the moments (see, e.g. [5,6]). The physical kinetics methodology was used for the analysis of simulation results. Bulk condensation was considered as a relaxation process (condensation relaxation) with characteristic time τ_c, which was determined as a time interval during which initial value of supersaturation ratio decreases by a factor of *e*. Use of such approach by analogy with second-order phase transitions made possible to obtain scaling correlations for the important characteristics of first-order phase transition, in particular numerical density of formed droplets n_d and time of condensational relaxation τ_c. Also it turned out to be possible to take into account disturbances of thermodynamic parameters of process (temperature and pressure) relative to average values. It was noted that some time interval existed in beginning of condensation relaxation, during which new droplets formed with constant nucleation rate at nearly constant values of temperature and supersaturation ratio. This time interval was called the induction period τ_i by analogy to combustion theory. Relation between the induction period and the nucleation rate was established at initial values of temperature and supersaturation ratio. In opinion of authors of [3], obtained relations give a principal possibility for experimental determination of nucleation rate one more method. As against many existing methods [7], it can allow to determine the nucleation rate at that stage when nucleating droplets cannot be detected by optical methods.

This paper has the following structure. The problem formulation for condensation relaxation of supersaturated vapor in a mixture with non-condensing gas is presented in Section 2. Also the appropriate system of the equations is presented in Section 2. In Section 3, the new method offered by authors for solving the kinetic equation for droplet size distribution function is described. In Section 4, the results of application of the method offered by authors are submitted, and the comparative analysis is given for obtained results and the solution of the same problem with use of a method of the moments. The basic deductions on work are given in Section 5.

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Nomenclature

C_p	specific heat
D	diffusion coefficient
f	droplet size distribution function
F	velocity distribution function of molecules
g	mass fraction
I	nucleation rate
J	the collision integral
Kn	Knudsen number
L	evaporation heat
n	number density
N_{A}	Avogadro number
p	pressure
r	droplet radius
$\dot{r}$	droplet growth rate
R	the universal gas constant
s	supersaturation ratio
t	time
T	temperature
v_{T}	thermal velocity of molecules
V	volume

Greek symbols

α	condensation coefficient
γ	adiabatic index
λ	mean free path of molecules
μ	molar mass
ξ	molecular velocity
ρ	density
Ω	moment of distribution function

Subscripts and superscripts

cr	critical radius
d	parameter of droplets
i	node number in the droplet radius grid
j	time step number
l	parameter of liquid
n	order of moment
s	parameter in state of saturation
v	parameter of vapor
Σ	parameter of vapor–gas–droplets mixture

2. Formulation of the relaxation problem

We considered a mixture of vapor and incondensable gas in an adiabatically isolated cylinder with a moving plunger. At the initial time moment, the vapor is in a steady state at the saturation. Then plunger begins to move, and the velocity of plunger governs the rate of the vapor–gas mixture expansion and the rate of the vapor supersaturation development. The motion of plunger in turn determines the degree of the expansion (the ratio of current volume V to initial volume V_0) and the vapor supersaturation ratio $s = p_{\mathrm{v}}/p^{\mathrm{s}}_{\infty}(T)$, where $p^{\mathrm{s}}_{\infty}(T)$ is the saturation pressure over a flat vapor–liquid interface. It was shown in [4] that the supersaturation ratio can be found from following equation:

$$\frac{\mathrm{d}\ln s}{\mathrm{d}t} = A_1\frac{\mathrm{d}\ln V}{\mathrm{d}t} - \alpha\pi r_{\mathrm{d}}^2 n_{\mathrm{d}} v_{\mathrm{T}} A_2. \tag{1}$$

Here

$$A_1 = (\gamma-1)\left(\frac{L\mu_{\mathrm{v}}}{RT} - \frac{\gamma}{\gamma-1}\right), \quad A_2 = 1 + g_{\mathrm{v}}\frac{L}{C_pT}\left(\frac{L\mu_{\mathrm{v}}}{RT} - 1\right), \tag{2}$$

where γ is the adiabatic index, L is the heat of evaporation, C_p is the specific heat of the vapor–gas–droplet mixture, v_{T} is the thermal velocity of vapor molecules, g_{v} is the vapor mass fraction in the mixture, n_{d} is the droplet-number density, and r_{d} is the average droplet size.

The first term in right part of (1) describes increase of the supersaturation ratio due to the adiabatic expansion, while the second one describes decrease of the supersaturation ratio due to vapor phase depletion (the first term in A_2) and to an increase in the temperature caused by the heat of the phase transition (the second term in A_2). Eq. (1) was obtained with use of definition of the supersaturation ratio, the temperature dependence of the saturation pressure according to the Clausius–Clapeyron equation, the Poisson adiabatic equation, and the vapor state equation, as well as the balance equations for energy and number of vapor molecules:

$$\rho_{\Sigma}C_p\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{L\mu_{\mathrm{v}}}{N_{\mathrm{A}}}\frac{\mathrm{d}n_{\mathrm{c}}}{\mathrm{d}t}, \tag{3}$$

$$\frac{\mathrm{d}n_{\mathrm{c}}}{\mathrm{d}t} = -\frac{\mathrm{d}n_{\mathrm{v}}}{\mathrm{d}t}. \tag{4}$$

Also it was taken into account that number of vapor molecules decreased due to their collision with droplets with probability α:

$$\frac{\mathrm{d}n_{\mathrm{v}}}{\mathrm{d}t} = -\alpha\pi r_{\mathrm{d}}^2 V_{\mathrm{T}} n_{\mathrm{d}} n_{\mathrm{v}}. \tag{5}$$

Here n_{v} and n_{c} are the number densities of vapor and condensate molecules, respectively, and N_{A} is Avogadro number. It should be noted that use of united energy balance equation for both phases in the form (3) is possible if temperature of droplets is equal to one of vapor–gas mixture. We call this case further as one-temperature model [2]. This model was used in this paper as well as in [2–4], and this allowed comparing obtained results.

At such an approach, it is quite possible to account for that fact that the heat release during condensation occurs on the surface of growing droplets followed by the heat transfer to the gaseous phase at a finite rate. In this case, droplets turned out to be superheated compared with the vapor, thus retarding the processes of droplet nucleation and growth. The limits of the variations in droplet temperature are known. At the lower limit, this is the temperature that is identical for both phases. At the upper limit this is the saturation temperature corresponding to the vapor pressure above droplet (the "Oswatitsch assumption"). The one-temperature model is closer to the real situation the higher the vapor dilution with non-condensing gas and the lower the coefficient of condensation. Otherwise, the "Oswatitsch assumption" is close to reality.

The value of $n_{\mathrm{d}}r_{\mathrm{d}}^2$ in Eq. (1) is virtually the second moment of droplet size distribution function. For this reason system of equations, which describes process of condensational relaxation, should include corresponding equation for distribution function. This equation has the following form (see, e.g. [5,6]) for homogeneous condensation in an immovable medium without coagulation of droplets:

$$\frac{\partial f}{\partial t} + \frac{\partial(\dot{r}f)}{\partial r} = \frac{I}{\rho_{\Sigma}}\delta(r - r_{\mathrm{cr}}). \tag{6}$$

Here f is the mass distribution function of droplet sizes, r is the droplet radius, $\dot{r}$ is the droplet growth rate, I is the nucleation rate, ρ_{Σ} is the density of the vapor–gas–droplets mixture, δ is the delta function, and r_{cr} is the critical droplet radius.

If volume condensation is studied, and then overall characteristics of process are of interest usually. Numerical density of droplets, their average size, mass or volume fraction of liquid can be