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Evaporation in mixture of vapor and gas mixture

A.P. Kryukov *, V.Yu. Levashov, I.N. Shishkova

Department of Low Temperatures, Moscow Power Engineering Institute, Krasnokazarmennaya 14, Moscow 111250, Russia

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ABSTRACT

The evaporation problem in vapor and gas mixture is investigated by the methods of molecular-kinetic theory and fluid dynamics. Solution results are obtained for the case when investigation domain length is several thousands mean free paths of molecules. In this statement two types of evaporation problem solutions are obtained. In the first type gas is completely pushed up by vapor from the region near the evaporation interface surface. In this, "shelf" (straight step) in dependence of vapor density on coordinate takes place. In the second type such "shelf" is not formatted. Transition from one type solution to another is found.

1. Introduction

It is well known that the intensity of transfer processes at evaporation and condensation depends strongly on the presence of a non-condensable gas in vapor and gas mixture. This effect is confirmed by different calculations [1,2] and experimental research data [3,4]. For example in [2] the condensation process on interface surface is studied for one-dimensional statement when vapor flowed from semi-infinite space through the binary vapor and gas mixture. In this paper it was concluded that condensation is possible in principle only if the quantity of gas in system is smaller in some limited value. Thus non-condensable component can lock up the interface surface and condensation stops completely. A similar behavior was noted early by Aoki and co-authors in [1] on the study of vapors flows caused by evaporation and condensation on two parallel plane surfaces in the presence of a non-condensable gas.

Sometimes the role of non-condensable gas can be very important. For example: in [3] experimental study of the condensation of mercury the small enough pressures were realised. In [4] the concentration of background gas pressure was in five times smaller than that in the previous paper. In these conditions the corresponding mass flux densities at condensation processes differ from each other by 15–20%.

The evaporation and condensation problems for pure vapor and in semi-infinite statement have been studied by different authors [5–11]. For example in [5] the solutions of one-dimensional weak evaporation and condensation problems in a semi-infinite space were reported. The authors of this paper obtained the following expression for the intensity of evaporation and condensation processes:

$$j = \frac{\beta}{1-0.4\beta}\left(\rho_s\sqrt{\frac{RT_s}{2\pi}} - \rho_\infty\sqrt{\frac{RT_\infty}{2\pi}}\right), \tag{a}$$

where β – evaporation (condensation) coefficient. This expression can be used in the case when vapor flow Mach number is much smaller the unit (weak evaporation). Weak condensation problem from space contained vapor and gas mixture on the base of kinetic theory was investigated in [6].

In [7–10] strong evaporation and condensation of pure vapor have been studied. For the case when intensity evaporation and condensation can be arbitrary the following expression for evaporation intensity at $\beta = 1$ is presented in [9]:

$$j = 0.6\sqrt{2RT_s}(\rho_s - \rho_\infty)\sqrt{\frac{\rho_\infty}{\rho_s}} \tag{b}$$

The problem becomes more difficult in the case when investigation domain is occupied by a mixture of vapor and non-condensable component. The results of problem solution in this case are presented in [11] for some sets of component masses and concentrations relation. These results were received as evolution of [9] approach.

In the present article, we have used method of joint solution of the Boltzmann kinetic equations (BKEs) system and system of Navier and Stokes equations (NSEs). In this approach the study of mixture flows near surfaces is based on the BKEs system. Mixture flow outside these regions is described by fluid dynamic equations (NSEs).

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* Corresponding author. Tel.: +7 495 3627841; fax: +7 495 3627215.
E-mail address: KryukovAP@mpei.ru (A.P. Kryukov).

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Nomenclature

C_g	mass concentration of gas component
D	diffusion coefficient
e	internal mixture energy
f	molecular velocity distribution function
h	enthalpy of component
j	mass flux density
j^{diff}	diffusion mass flux
$J_{\phi\psi}$	collision integral
$K_n = \lambda/L$	Knudsen number
L	investigation domain length
m_v	mass of vapor molecule
m_g	mass of gas molecule
n	numerical density
p	mixture pressure
q	energy flux
R	gas constant for vapor
T	temperature
$t^{dimension}$	dimension time
t	dimensionless time
u	mixture velocity
x	coordinate

Greek symbols

λ	mean free path of vapor molecules
λ_T	thermal conductivity of mixture
β	evaporation (condensation) coefficient
μ	mixture viscosity
ξ	molecular velocity
ρ	mixture density
ρ_s	saturated of vapor density corresponding to T_s
ρ_v	density of vapor component
ρ_g	density of gas component

Subscripts

v	vapor component
g	gas component
s	surface
base	base parameters
∞	away from evaporation and condensation surface (outside Knudsen layer)

2. Problem and solution method

Evaporation from interface surface in space occupied by a mixture of vapor (water, as example) and non-condensable gas (nitrogen, as example) is considered. Statement of this problem is presented in Fig. 1.

Calculative domain is limited on the left-hand side by interface surface. Temperature of this surface is T_1; numerical density of vapor molecules corresponding to this temperature along saturation line is n_{v1}. At the initial time moment all investigated domain is occupied by vapor and gas mixture with numerical densities vapor and gas n_{v0}, n_{g0} correspondingly and temperature $T_0 = T_1$. Velocity distribution functions at the initial moment are prescribed by Maxwell's distributions with temperature T_0, corresponding numerical densities and zero mean (macroscopic) velocities.

It is assumed in real physical situation that calculative domain is not limited on the right-hand side as shown in Fig. 1. At numerical investigation there is no possibility to obtain solution namely in semi-infinite space. Therefore in the present paper the size of calculative domain is taken large enough along x coordinate in order to avoid the disturbance influence of right boundary on the vapor and gas flows near interface surface during the time of solution evolution. In presented cases domain with size about in the range of 25,000 – 50,000 λ_{base} is considered depending on concrete initial and boundary conditions, where λ_{base} – mean free path of water molecules at base parameters of problem.

Base parameters are assumed as temperature $T_{base} = T_1$ and numerical density of water molecules n_{vbase}, corresponding to T_{base} along saturation line. The ratio of component molecular masses is 0.64, the ratio of diameters is 1.25. At $x \to \infty$ the following mixture parameters are given: temperatures $T_2 \approx T_1$, numerical densities of vapor n_{v2} and gas molecules $n_{g2} = n_{g0}$. Approximation of equality $T_2 \approx T_1$ should be understood as follows. Let us believe that vapor is water vapor. Hence interface surfaces are the surfaces of water. If, for example, $T_1 \approx 340$ by Kelvin (67 °C) and $T_2 \approx 324$ by Kelvin (51 °C), then corresponding to these temperatures saturation pressures are $p_1 \approx 27354$ Pa and $p_2 \approx 12973$ Pa. Thus the pressure ratio is $p_1/p_2 \approx 2.1$ and temperature ratio is $T_1/T_2 = 1.05$, that is $T_1 \approx T_2$.

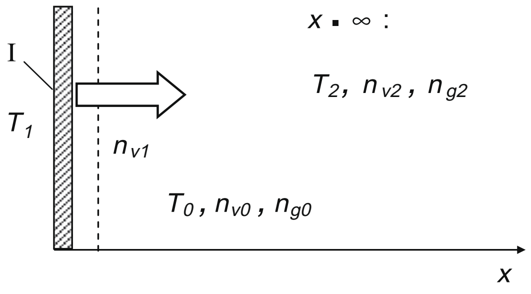

Fig. 1. Statement of the problem.

All molecules incident on interface surfaces (limited surfaces) condense on these surfaces. From these surfaces evaporation takes place: n_{v1} и n_{v2} – numerical densities of vapor (water) molecules incoming in the calculative domain from limited surfaces. Diffuse type of evaporation is assumed. For gas component both boundaries are impenetrable and reflection is described by diffuse scheme also. All boundary velocity distribution functions are semi-Maxwell's distributions with the corresponding temperature, numerical densities and zero mean (macroscopic) velocities.

As well known too much computer time is required for the solution of the BKEs system (1) for large calculating range (more than 100 length of the mean free paths for the vapor molecules). As followed in this work the technique of joint solution [12] of kinetic equations system and fluid dynamic equations is used for the investigation of evaporation and condensation problem. In this approach system (1) is solved in thin domains that adjoin to the surfaces of evaporation (I) (the length of this domain is a few mean free paths of vapor molecules). Mixture flows outside these thin regions are described by fluid dynamic equations (Navier and Stokes) (2). In this case the results of the BKE solution are used as boundary conditions for Navier and Stokes equations. This approach gives the possibility to decrease the computer time and to extend the investigated domain.

The Boltzmann kinetic equations system for gas mixtures [13]:

$$\begin{aligned} &\frac{\partial f_v}{\partial t} + \xi_v \frac{\partial f_v}{\partial x} = J_{vv} + J_{vg}, \\ &\frac{\partial f_g}{\partial t} + \xi_g \frac{\partial f_g}{\partial x} = J_{gv} + J_{gg}, \end{aligned} \tag{1}$$

where $f_v = f_v(x, t, \xi_v)$ and $f_g = f_g(x, t, \xi_g)$ – distribution functions for vapor («v») and gas («g») component accordingly, x – coordinate,

$\xi = (\xi_x, \xi_y, \xi_z)$ – molecular velocity, $J_{\varphi\psi}(\phi = v,g;\ \psi = v,g)$ – collision integrals.

Numerical method for solution (1) and the results of corresponding tests are presented in [14].

System of fluid dynamic equations can be presented as following [15]:

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0, \quad \frac{\partial \rho_g}{\partial t} + \frac{\partial \rho_g u}{\partial x} + \frac{\partial j_g^{diff}}{\partial x} = 0 \\
&\frac{\partial \rho u}{\partial t} + \frac{\partial}{\partial x}(\rho u^2) = -\frac{\partial p}{\partial x} + \frac{4}{3}\frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial x}\right) \\
&\frac{\partial \rho e}{\partial t} + \frac{\partial \rho e u}{\partial x} = -p\frac{\partial u}{\partial x} + \frac{4}{3}\mu\left(\frac{\partial u}{\partial x}\right)^2 - \frac{\partial q}{\partial x},
\end{aligned} \tag{2}$$

where $\rho = \rho_v + \rho_g$ – mixture density, $\rho_g = m_g n_g$, $\rho_v = m_v n_v$ – densities of «v» and «g» components accordingly, p – mixture pressure, $j_g^{diff} = -\rho D \frac{\partial C_g}{\partial x}$ – diffusion mass flux, $C_g = \rho_g/\rho$ – mass concentration of «g» component, D – diffusion coefficient, $q = -\lambda_T \frac{\partial T}{\partial x} + (h_g - h_v) j_g^{diff}$ – energy flux in binary mixture, h_v и h_g – enthalpy of component, λ_T – thermal conductivity of mixture, e – internal mixture energy, μ – mixture viscosity, m_v and m_g – molecular masses of «v» and «g» component accordingly.

The fluid is assumed to be ideal gas. The model of hard elastic spheres was used for the calculation of viscosity, thermal conductivity and diffusion coefficients. Also other correlations for the calculations of transport coefficients presented in [16] have been

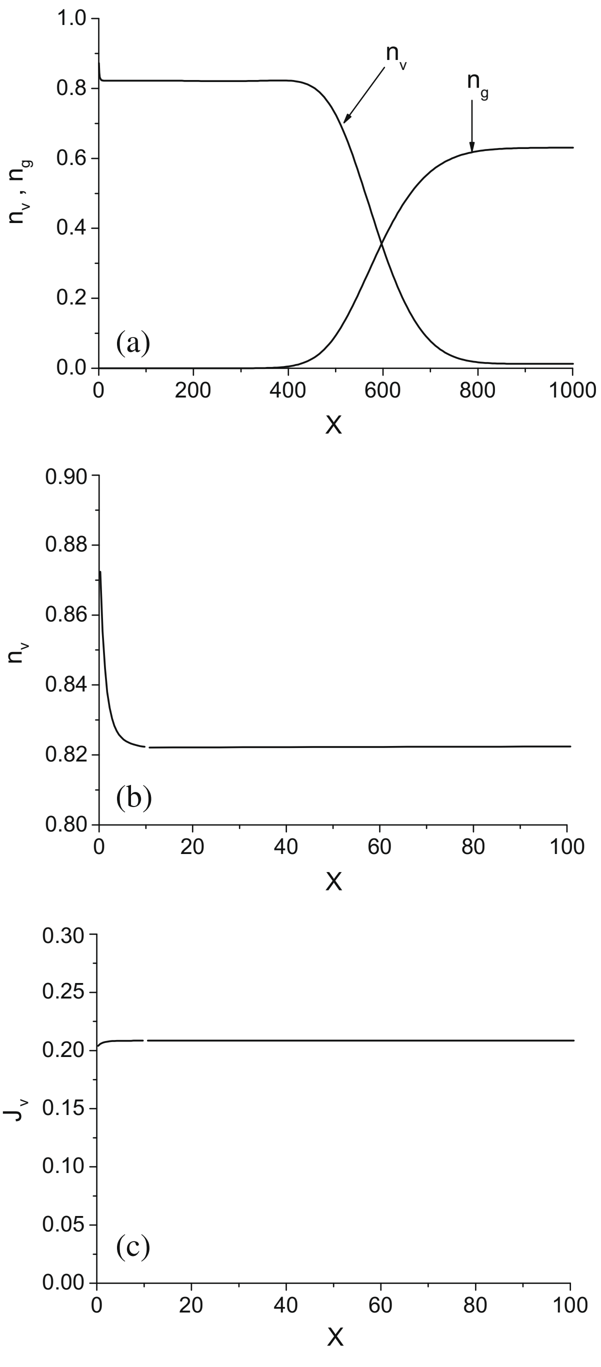

Fig. 2. Solution results for $n_{v1} = 1.1$, $n_{v2} = 0.01$, $n_{g0} = 0.5$; (a) vapor and gas density, (b) vapor density, and (c) vapor mass flux density.

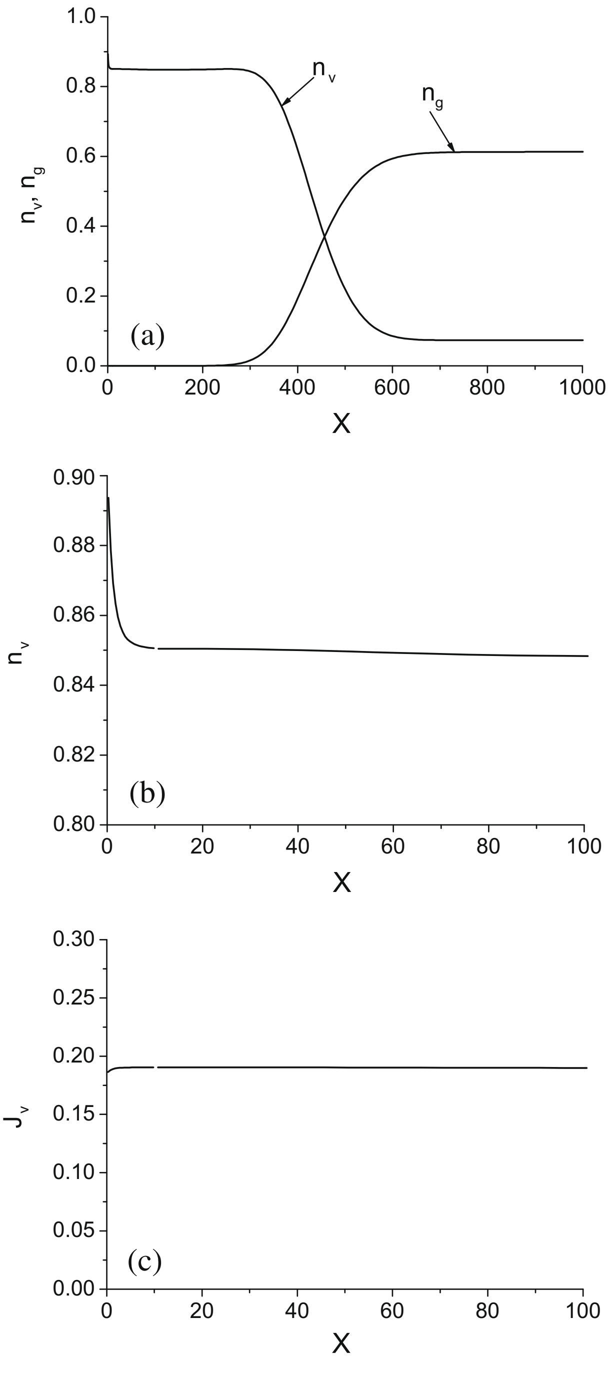

Fig. 3. Solution results for $n_{v1} = 1.1$, $n_{v2} = 0.06$, $n_{g0} = 0.5$; (a) vapor and gas density, (b) vapor density, and (c) vapor mass flux density.

made. In this in accordance with [16] the difference of the corresponding coefficients values is not more than 4%. It should be noted that solution method used in our present paper gives the possibility to use different types of gas (vapor) molecules interaction potentials, for example Lennard–Jones interaction.

3. Results and analysis

Solution results of the evaporation and condensation problem in semi-infinite space (in the sense described above) for the different contents of non-condensable component and various initial concentrations of vapor are shown in Fig. 2–6. All solutions were obtained for $T_0 = T_1$. Results of the evaporation and condensation problem in semi-infinite space (in the sense described above) for the different contents of non-condensable component are shown in these figures in a dimensionless form as dependences on coordinate x. At this: $n'_v = n_v/n_{vbase}, n'_g = n_g/n_{vbase}$, $x' = x/\lambda_{base}$, $j'_v = j_v/(mn_{vbase}(RT_{base})1/2)$. Further everywhere primes are omitted.

Submitted in these figures are the distributions obtained as a result of the non-steady problem solution. Lines presented in these Figures are depicted for time moment when changing density and mass flux density for vapor and gas in the region near interface surface ceased. At this length of such region in accordance with problem solutions is about four hundred mean free paths. It is seen from these figures that near the inter-phase surface thin layer of $5 \div 10\lambda$ in size is formed, in which appreciable change of macroparameters is observed. Outside this layer, i.e. at $x > 10\lambda$, macroparameters are constant right up large enough distance from interface surface (about four hundred mean free paths, as example).

It is interesting to note, that such steady solutions essentially depend on not only from presence in domain non-condensable component, but also on the vapor quantity contained in this area at the initial moment of time. So if to compare the results of Figs. 2 and 3, it is possible to see, that in both cases gas is pushed out by vapor on distance about hundreds mean free path of water molecules λ_{base} at $T_{base} = T_1$ and numerical density of water molecules n_{vbase}, corresponding to T_{base} in accordance with the saturation line. However the "stationary"(or more correctly "quasi- stationary") vapor density for a case $n_{v2} = 0.01$ makes 0.82, while for a case when initial vapor density is more in 6 times, i.e. $n_{v2} = 0.06$ the

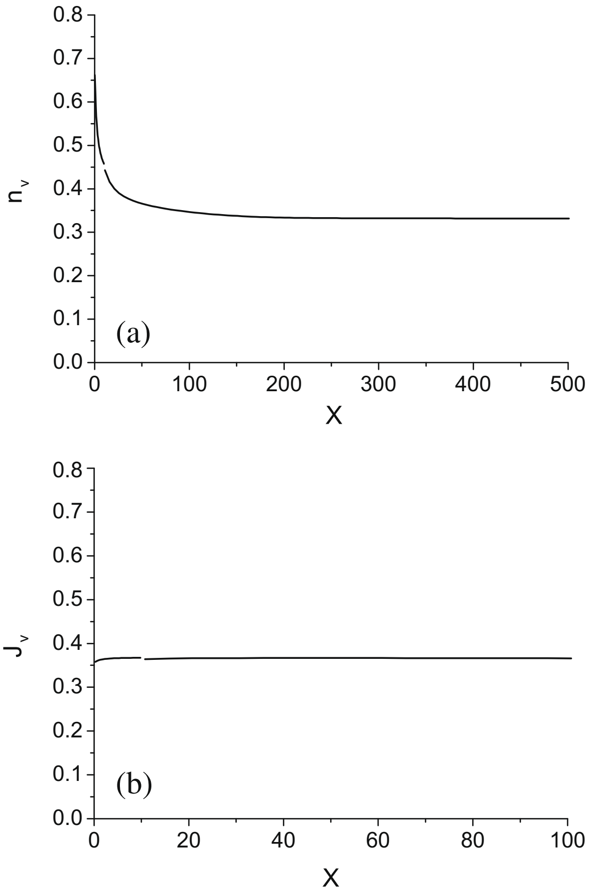

Fig. 4. Solution results for $n_{v1} = 1.1$, $n_{v2} = 0.06$, $n_{g0} = 0.0$; (a) vapor density and (b) vapor mass flux density.

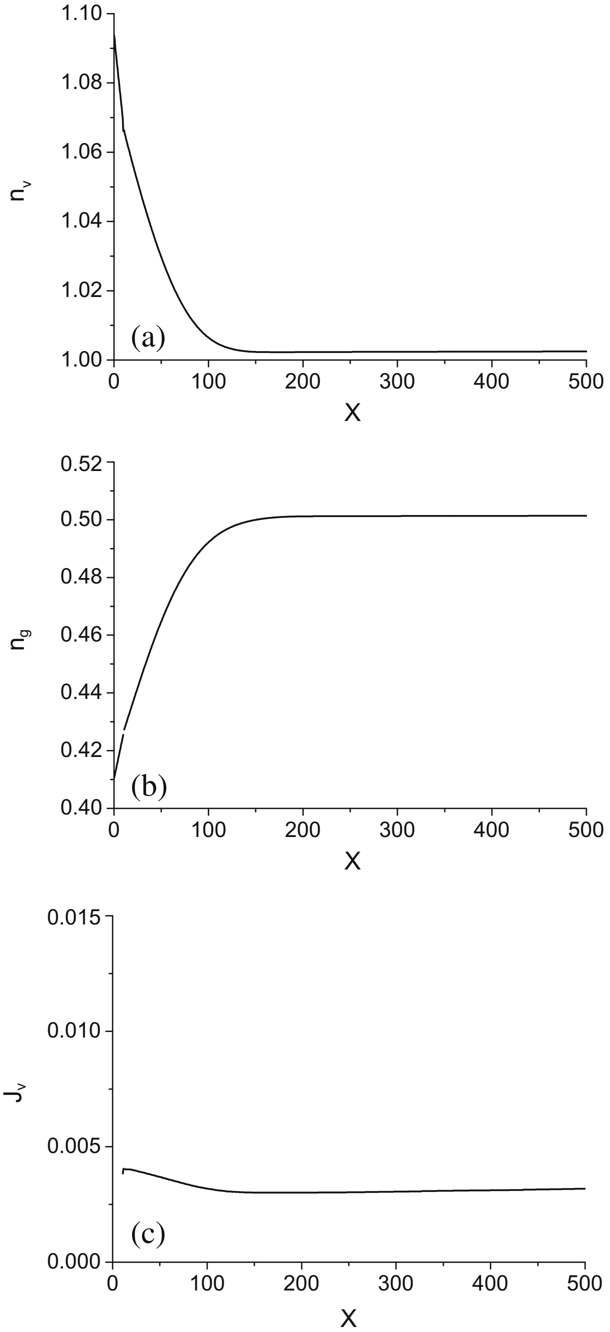

Fig. 5. Solution results for $n_{v1} = 1.1$, $n_{v2} = 1.0$, $n_{g0} = 0.5$. (a) Vapor density, (b) gas density, and (c) vapor mass flux density.

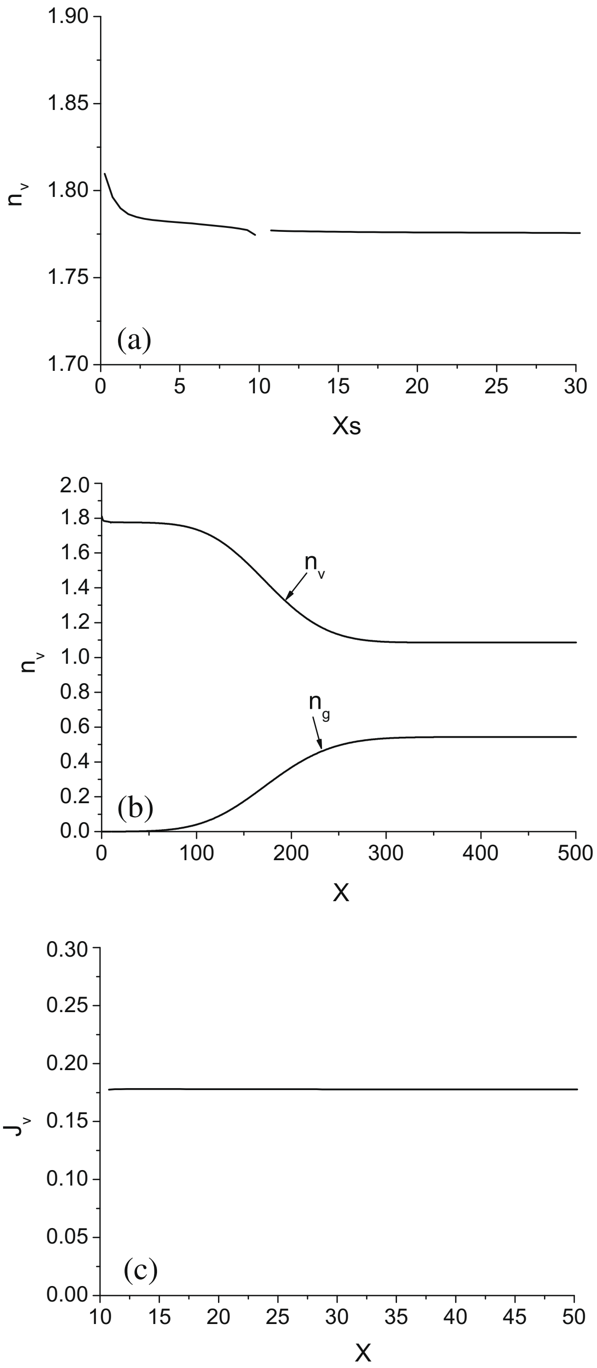

Fig. 6. Solution results for $n_{v1} = 2.0$, $n_{v2} = 1.0$, $n_{g0} = 0.5$; (a) vapor density, (b) vapor and gas density, and (c) vapor mass flux density.

“stationary” vapor density is 0.85. Vapor mass flux densities in both cases are close enough and make 0.21 and 0.19 accordingly.

It was noted above that solutions presented in Figs. 2 and 3 were obtained for evaporation and condensation problem in the presence of non-condensable gas. At this distance between evaporation and condensation inter-phase surfaces was about in the range of 25,000 – 50,000 mean free paths of water molecules λ_{base}. Solution results for analogous problem for clean vapor (without gas component) are presented in Fig. 4. Results shown in Figs. 2 and 3 are qualitatively similar with the data for evaporation and condensation problem in clean vapor (Fig. 4). However the comparison of Figs. 2–4 shows that the values of vapor and mass flux densities in mixture problems differ substantially from the corresponding values for clean vapor.

The discussed solutions are obtained as in and as out the thin limited layer. One can see in Fig. 2a or Fig. 3a that despite of existence of the steady behavior of macroparameters in the region adjoining to surface I, on large distance from it always it is possible to observe front of the solution width 300–500 λ_{base} where vapor and gas densities vary from one constant values up to others. Thus the solution actually represents a step extending along X coordinate. At the same time, there is such a ratio of the vapor and gas densities when the solution is qualitatively different. The densities (vapor and gas) are changed from the meanings close to given on interface surface up to the appropriate values at very far from it (Fig. 5). It occurs on the length of the order of several hundreds mean free paths λ_{base}.

If in the first two cases (see Figs. 2 and 3) the correlation $n_{v1} >> n_{v2}$ was valid, further was taken $n_{v1} \approx n_{v2}$ at the same value of initial density of gas n_{g0}: $n_{v1} = 1.1$, $n_{v2} = 1.0$, $n_{g0} = 0.5$ (Fig. 5). The solutions presented in Fig. 5 differ from those shown in Figs. 2 and 3. Change of the vapor density occurs in layer thickness almost $150\lambda_{base}$ instead of $5 \div 10\lambda_{base}$ in the previous problems (Fig. 5a). Complete pushing away from interface surface of the gas is not observed (Fig. 5b) because the intensity of evaporation is too small. The vapor mass flux density decreases almost in 70 times (Fig. 5c). These results show that the presence of non-condensable gas and initial quantity vapor in the investigated domain make essential influence on the character of solution.

A similar problem was solved at $n_{v1} = 2.0$, $n_{v2} = 1.0$, $n_{g0} = 0.5$. Results are presented in Fig. 6. From Fig. 6a one can see that the layer near the interface surface almost disappeared, more precisely the thickness of this layer became less than $2\lambda_{base}$ for vapor density. In this case the density increase near the interface surface ($x = 0$) was comparable with error calculations. As well as in the first two cases vapor pushes up gas from the interface surface in outside and value of mass flux density is great enough (about 0.18).

In order to study the influence of initial gas density on solution behavior the problem was solved at $n_{v1} = 1.1$, $n_{v2} = 0.06$ and different n_{g0}, namely in addition to $n_{g0} = 0.5$ (see above and Fig. 3) at $n_{g0} = 0.3$ and $n_{g0} = 0.1$.

Results are presented in Table 1 below. The following designations are used: n_v^* – vapor density according the “shelf” (straight step) in steady solution. In Table 1 the values n_v^* and vapor mass flux density j_v are given depending on n_{v1}, n_{v2} and n_{g0}.

From this table, first of all, the role of a non-condensable component in researched domain is well visible. The comparison of the solutions Line 1 (Fig. 2) and Line 4 shows the following: if the

Table 1
Solutions results.

No.	n_{g0}	n_{v1}	n_{v2}	n_v^*	j_v
1	0.5	1.1	0.01	0.82	0.21
2	0.3	1.1	0.01	0.68	0.29
3	0.1	1.1	0.01	0.46	0.36
4	0.	1.1	0.01	0.33	0.37
5	0.5	1.1	0.06	0.85	0.19
6	0.3	1.1	0.06	0.72	0.27
7	0.1	1.1	0.06	0.52	0.35
8	0.	1.1	0.06	0.33	0.36
9	0.	1.1	0.1	0.41	0.36
10	0.	1.1	0.3	0.64	0.30
11	0.1	1.1	0.5	0.24	0.19
12	0.5	1.1	1.0	1.002	0.002
13	0.1	1.1	1.0	1.01	0.009
14	0.05	1.1	1.0	1.02	0.017
15	0.	1.1	1.0	1.03	0.036
16	0.5	2.	1.0	1.78	0.18
17	0.	2.	1.0	1.50	0.37

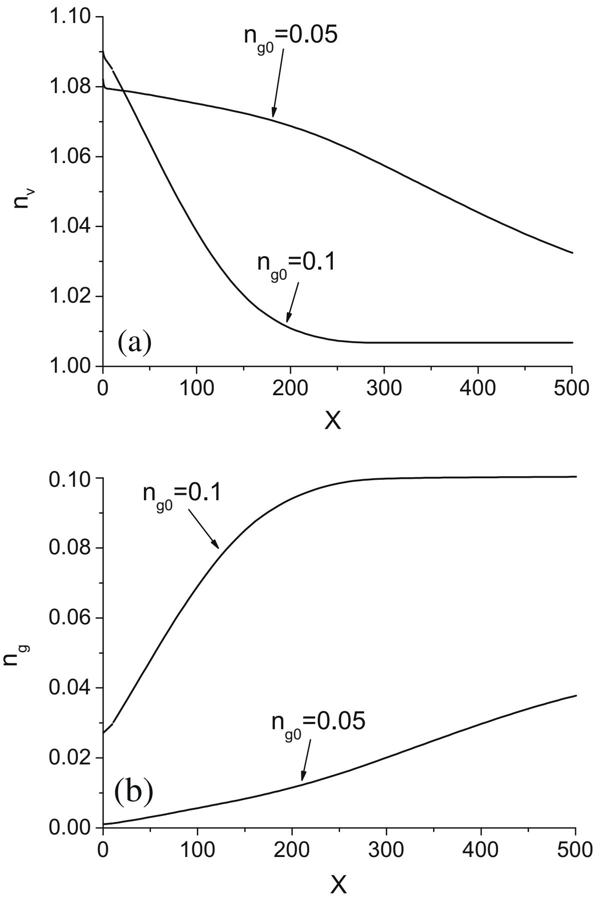

Fig. 7. Solution results for $n_{v1} = 1.1$, $n_{v2} = 1.0$, (a) vapor density and (b) vapor and gas density.

amount of the gas near the interface surface (evaporation surface I) equal zero then only vapor borders with interface surface. However the value of steady vapor density for case Line 1 (evaporation in vapor and gas mixture) is 2.5 times more than a similar value for case Line 4 (evaporation in pure vapor). Mass flux density of vapor for the case of evaporation in pure vapor (Line 4) is 1.7 times more than that for the case of evaporation in vapor and gas mixture (Line 1).

Comparison vapor and gas densities dependences on coordinate in Fig. 7 and the analysis of Lines 13 and 14 in Table 1 shows that at $n_{g0} \approx 0.05$ there is transition between two types of solution: with or without “shelf” near evaporation interface surface for $n_{v1} = 1.1$ and $n_{v2} = 1.0$.

4. Conclusions

The problem of evaporation in vapor and gas mixture has been investigated. At beginning of the study one-dimensional evaporation and condensation on plane interface surfaces statement was formulated. Distance between these surfaces was about $25000 \div 50000\lambda_{base}$. The technique of joint solution of the Boltzmann kinetic equations system and Navier and Stokes equations was used. This approach gave the possibility to decrease the computer time and to extend enough the investigated domain.

Solution results were obtained for the stage when disturbance from condensation interface surface did not appear in the calculative domain. Two solution kinds were revealed. In the first type gas was completely pushed up by vapor from the region near the evaporation interface surface. In this, “shelf” (straight step) in dependence of vapor density on coordinate took place. In the second type such “shelf” was not formatted. Transition from one solution kind to another at prescribed evaporation and condensation interface surfaces temperatures and corresponding vapor saturation densities is determined by the value of initial gas density. For concrete parameters this value (initial gas density at which transition between two types of solutions has place) was found approximately.

Acknowledgements

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