

# Evaporation-Condensation Problem In Vapour-Gas Mixtures

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**Abstract.** Evaporation-condensation problem concerning the strong-nonequilibrium vapour-gas mixture flow in nano- and micro- ducts is investigated. First part of this work develops the technique of numerical solution of the Boltzmann kinetic equations system for vapour-gas mixture. Next part is devoted to the technique of joint solution of kinetic equations system and fluid dynamic equations. Dependences of gas and vapour numerical densities and mass flux density on coordinate in one-dimensional problem for different vapour-gas mixtures are presented.

**Keywords:** evaporation, condensation, vapour-gas mixture, kinetic equations, fluid dynamic equations.

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At micro devices creation and nano-technologies the study of gas flows in ducts with typical sizes from micrometer to nanometer becomes valid. Moreover, in some cases the evaporation and condensation processes can take place on the duct boundary surfaces. At this non-condensable gas can be present in domain flow. As following, in the present paper the evaporation-condensation problem is considered for the case when domain length is about 100 mean free paths of vapour molecules (in this case Knudsen number ( $Kn$ ) is about 0.01). It is necessary to note that for pressure close to atmosphere condition this value ( $Kn = 0.01$ ) corresponds to the domain length near 5 – 10  $\mu m$  for different gases. If pressure increases in 10 times, this size should be 500 – 1000  $nm$ .

First part of this work develops the technique of numerical solution of the Boltzmann kinetic equation (BKE) for vapour-gas mixtures. The main attention is focused to the calculation of collision integrals for gas-gas, vapour-vapour, gas-vapour and vapour-gas interactions. This approach provides possibility to study interaction of mixture components of a various nature (diameters and masses of molecules can be different in wide range).

As well known too much computer time is required for the solution of the BKE system for large calculating range (more then 100 length of the mean free paths for the vapour molecules). As following, other part of this work is devoted to the technique of joint solution of kinetic equations system and fluid dynamic equations for the investigation of evaporation-condensation problem. At this approach whole investigation range is divided in the following parts: 1) kinetic region that adjoins directly to the surface of evaporation (condensation); 2) fluid dynamic equations region situated on distance of 10-20 mean free paths of vapour molecules from surface of evaporation (condensation). The study of mixture flows near surfaces is based on the BKE system. Mixture flow outside these thin regions are described by fluid dynamic equations (Navier-Stokes). In this case the results of the BKE solution are used as a boundary conditions for Navier-Stokes equations.

## PROBLEM AND SOLUTION METHOD

Evaporation-condensation problem in domain between two infinite interphase surfaces is considered. The statement of this problem is shown in Fig. 1. The evaporation of vapour (component «a») takes place at surface I. On the interphase surfaces (I and II) incident vapour molecules are absorbed completely. In the initial time moment ( $t = 0$ ) vapour (component «a») and gas (component «b») occupy domain I – II between two surfaces. The temperature of the both surfaces are approximately equal  $T_I \approx T_{II} \approx 1.0$ , but it is assumed that saturated vapour numerical densities  $n_{aI}$  and  $n_{aII}$  corresponding to temperature  $T_I$  and  $T_{II}$  differ in two times, i.e.  $n_{aI} = 2n_{aII}$ . The vapour

numerical density  $n_{all}$  and surface temperature  $T_{II}$  are used as parameters of the reference state. The co-ordinate  $x$  is given in the mean free paths of vapour molecules at these parameters ( $l$ ) and time  $t$  is given in relation to  $l/\sqrt{R_a T_{II}}$ , where  $R_a$  – individual vapour constant per unit mass ( $R_a = k_B/m_a$ ),  $k_B$  – the Boltzmann constant.

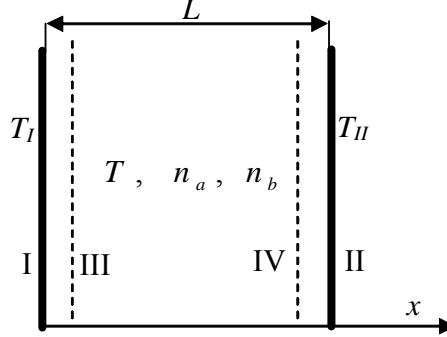


FIGURE 1. Schematic illustration of the problem.

The Boltzmann kinetic equations system for gas mixtures [1]:

$$\begin{aligned} \frac{\partial f_a}{\partial t} + \xi_a \frac{\partial f_a}{\partial x} &= J_{aa} + J_{ab}, \\ \frac{\partial f_b}{\partial t} + \xi_b \frac{\partial f_b}{\partial x} &= J_{ba} + J_{bb}, \end{aligned} \quad (1)$$

where  $f_a = f_a(x, t, \xi_a)$  and  $f_b = f_b(x, t, \xi_b)$  – distribution functions for «a» and «b» component accordingly,  $x$  – co-ordinate,  $\xi = (\xi_x, \xi_y, \xi_z)$  – molecular velocity,  $J_{\varphi\psi}$  ( $\varphi = a, b$ ;  $\psi = a, b$ ) – collision integrals.

It is assumed that both vapour (component «a») as gas (component «b») consist of hard elastic spheres.

Once the values of the distribution function in various points in the physical space and at a certain moment of time are found, we can calculate by the integration in velocity space such moments of these functions as numerical densities of gas or vapour, mass flux density in the direction  $x$  and others.

Our numerical algorithm is based on the method of direct numerical solution of the Boltzmann equation, described in [2]. It includes the following steps. Physical and velocity spaces are discretized along with time. The discretization of the velocity space is performed similarly to the physical space via replacing continuous values of  $\xi$  by a discrete set  $\{\xi^k\}^M$ , where  $k$  indicates the position of a velocity cell,  $M$  is the total number of cells. The

boundaries of the velocity domain in  $\xi_x, \xi_y, \xi_z$  directions are chosen in such a way that the contribution of molecules with velocities outside this range can be ignored.

For each value of  $\xi^k$ , the corresponding value of  $f(\xi^k)$  is specified. This allows us to present Equations (1) for each gas component in a discretized form:

$$\left\{ \frac{\Delta f_a}{\Delta t} + \xi_a^k \frac{\Delta f_a}{\Delta \mathbf{r}} = J_{aa}^k + J_{ab}^k \right\}^M, \left\{ \frac{\Delta f_b}{\Delta t} + \xi_b^k \frac{\Delta f_b}{\Delta \mathbf{r}} = J_{ba}^k + J_{bb}^k \right\}^M. \quad (2)$$

Following [2], the numerical solution of systems (2) is performed in two steps. Firstly, molecular displacements are calculated ignoring the effect of collisions. Secondly, the collisional relaxation is calculated at the assumption of spatial homogeneity.

The conventional approach to collisional integrals calculating is replaced by the integration based on random cubature formulae [2]. One of the used approaches for choosing random nodes is based on the Korobov sequences [2]-[4]. Using these sequences instead of random numbers makes it possible to reduce errors of computations.

The distribution of molecular velocities after collisions in this paper is found based on the assumption that 1) the total momentum and energy of colliding molecules are conserved; 2) the values of these momentums belong to grid notes. The second assumption was not used in the original method developed in [2]. Our approach have some similarities with the approaches used in [5]-[7] but the details are different [8]. Number of the collision combinations in this model is relatively small. Hence, in the practical implementation, the calculations were performed for all possible values for each collision and then the results were averaged over these variables.

System (1) is solved in thin domains that adjoin to the surfaces of evaporation (I) and condensation (II) (the length of this domain is a few mean free paths of vapour molecules). The boundaries of these domains (III and IV) are designated by dotted lines in Fig. 1. System of fluid dynamic equations is used for study of domain between III and IV. In one-dimensional non-steady statement this equations can be presented as following [9]:

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

where  $\rho = \rho_a + \rho_b$  – mixture density,  $\rho_b = m_b n_b$ ,  $\rho_a = m_a n_a$  – densities of «a» and «b» components accordingly,  $p$  – mixture pressure,  $j_b^{diff} = -\rho D \frac{\partial C_b}{\partial x}$  – diffusion mass flux,  $C_b = \rho_b / \rho$  – mass concentration of «b» component,  $D$  – diffusion coefficient,  $q = -\lambda_T \frac{\partial T}{\partial x} + (h_b - h_a) j_b^{diff}$  – energy flux in binary mixture,  $h_a$  и  $h_b$  – enthalpy of component,  $\lambda_T$  – thermal conductivity of mixture,  $e$  – internal mixture energy,  $\mu$  – mixture viscosity,  $m_a$  and  $m_b$  – molecular masses of «a» and «b» component accordingly.

The fluid is assumed to be ideal gas. The model of hard elastic spheres was used for calculation of viscosity, thermal conductivity and diffusion coefficients.

The splitting principles at physical processes [9] are used for solution of system (3). In this case at the first stage the system (3) is solved without taking into account viscosity, heat conductivity and diffusion flux (Initial Euler stage). Solution of this system is based on the SHASTA algorithm [10].

At the following stage influence of viscosity, heat conductivity and diffusion fluxes are taken into account (Final Navie-Stokes stage). At this the implicit scheme is used for approximation of corresponding system. It should be emphasized that the values obtained by solution at the first stage (Initial Euler stage) are used as initial conditions for second stage (Final Navie-Stokes stage).

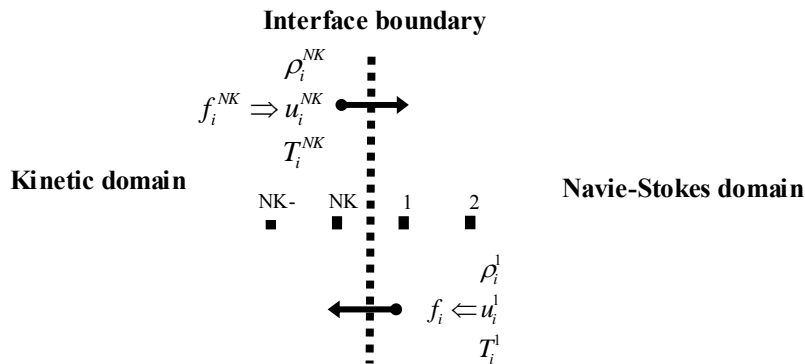


FIGURE 2. Schematic of joint solution procedure

The main part of the present work is devoted to the technique of joint solutions of system (1) and (3). The schematically this procedure is presented in the Fig. 2. The Chapmen-Enskog function with parameters from first

calculation point of Navie-Stokes domain –  $\rho_i^l, u_i^l, T_i^l$  ( $f_i = f(\rho_i^l, u_i^l, T_i^l)$ ,  $i=a,b$ ) is used for the velocity distribution function of molecules moved into kinetic domain –  $f_i$ . After solution of the kinetic system (1) velocity distribution function for each mixture component is found for whole kinetic domain. Macroparameters: density, temperature, pressure, mass flux, energy flux and others are calculated as moments of the distribution functions. Further system (3) is solved. At that, boundary conditions for this system are macroparameters from NK point.

In the present work “Interface boundary” (dotted lines in Figure 2.) are placed in distance of 10 mean free paths of vapour molecules from interface surfaces (I and II).

## RESULTS AND DISCUSSION

At the beginning presented above method was tested on the problem about evaporation-condensation of pure substance (one component system). In the initial time moment ( $t = 0$ ) domain between two surfaces is occupied by only vapour with numerical density  $n_a = 1.0$  and temperature  $T=1.0$ . The concentration of other component is equal 0, i.e.  $n_b = 0$ . Scheme of the problem is presented in Fig 1. The domain length ( $L$ ) is 100 mean free paths of vapour molecules. It is assumed that vapour molecules emitted by interphase surfaces have Maxwell distribution functions with  $T_I, n_{aI}, T_{II}, n_{aII}$ . It was supposed that  $n_{aI} = 2n_{aII}$  and  $T_I \approx T_{II}$ . The results of solution are presented in Fig. 3.

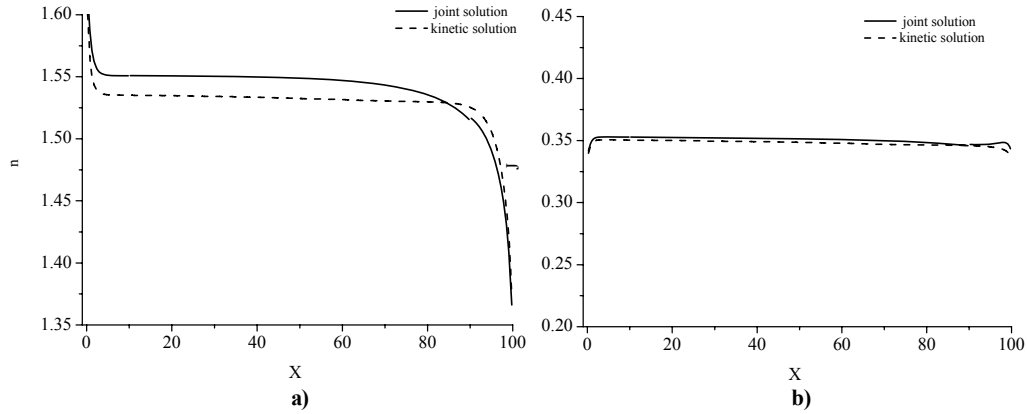


FIGURE 3. Dependence of vapour density  $n$  (a) and mass flux density  $J$  (b) on co-ordinate

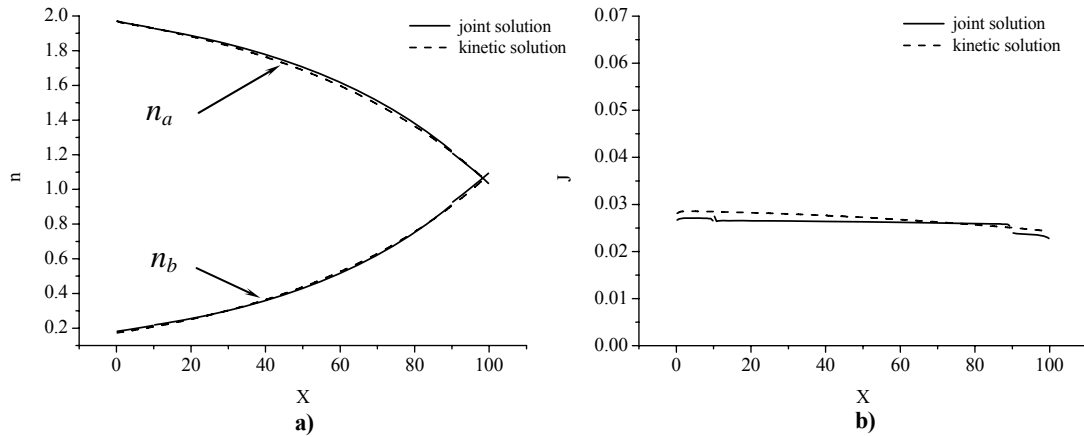
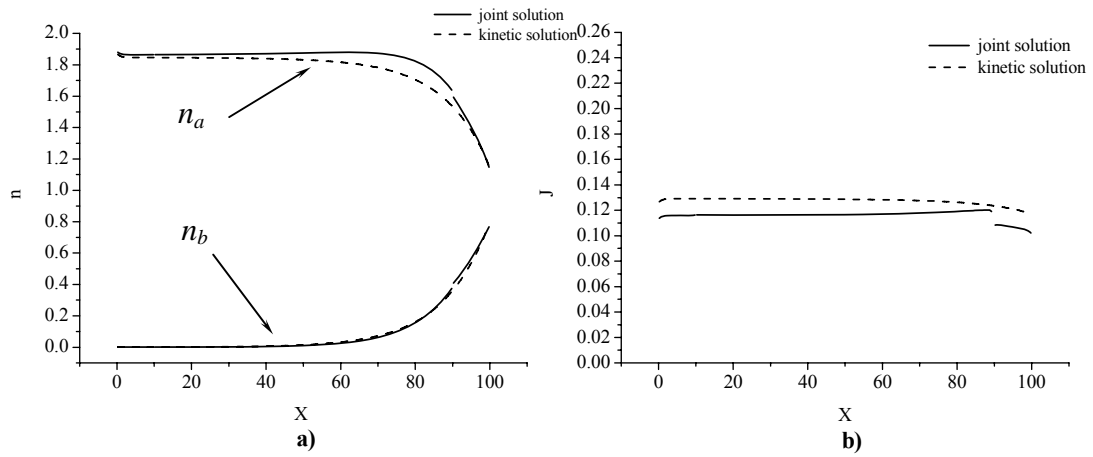
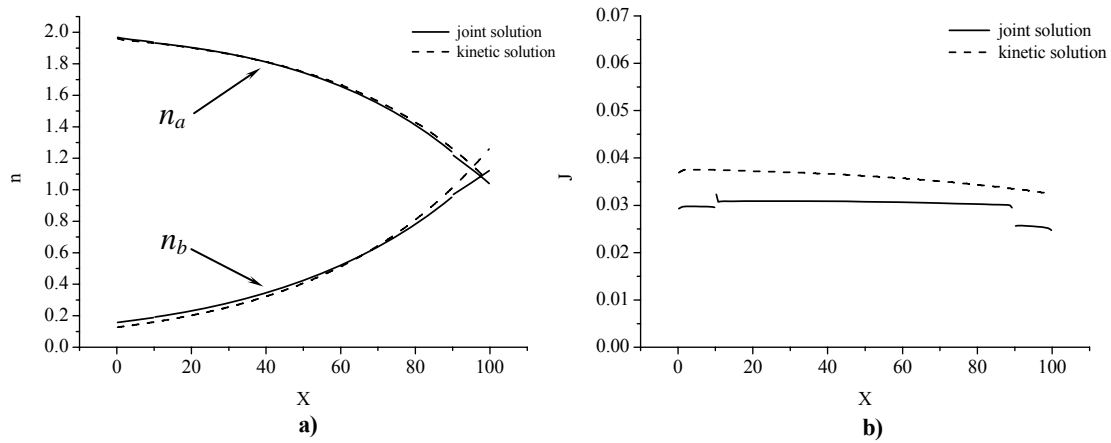


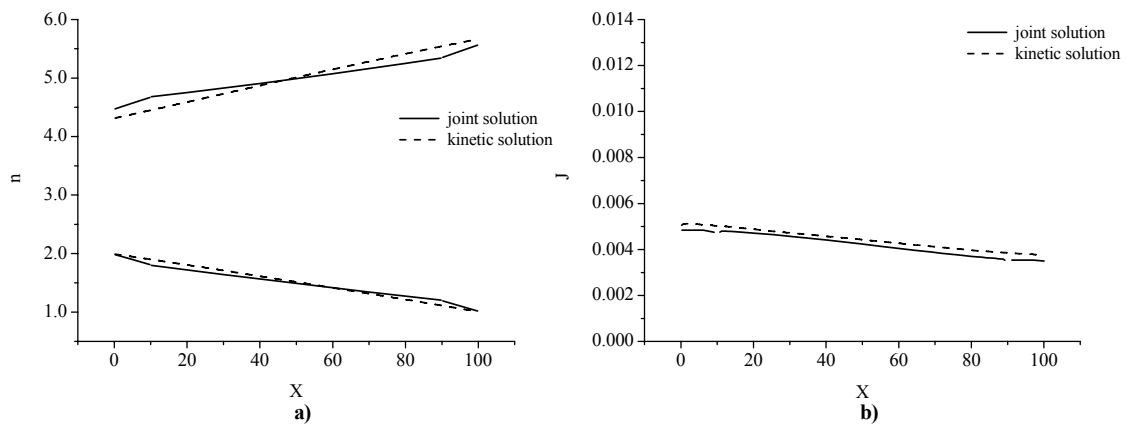
FIGURE 4. Dependence of vapour and gas densities (a) and mass flux density (b) on co-ordinate for case of mechanically identical molecules for case  $n_b = 0.5$



**FIGURE 5.** Dependence of vapour and gas densities (a), mass flux density (b) on co-ordinate for case  $n_b=0.1$  ( $m_a/m_b = 18/28$ ,  $d_a/d_b = 4.6/3.7$ )



**FIGURE 6.** Dependence of vapour and gas densities (a), mass flux density (b) on co-ordinate for case  $n_b=0.5$  ( $m_a/m_b = 18/28$ ,  $d_a/d_b = 4.6/3.7$ )



**FIGURE 7.** Dependence of vapour and gas densities (a), mass flux density (b) on co-ordinate for case  $n_b=5.0$  ( $m_a/m_b = 18/28$ ,  $d_a/d_b = 4.6/3.7$ )

Here and further below numerical densities and mass flux density are given in dimensionless form as  $n_b = n_b^D / n_{aII}$ ,  $n_a = n_a^D / n_{aII}$ ,  $j = j^D / (n_{aII} m_a \sqrt{R_a T_I})$ , where  $n_a^D$ ,  $n_b^D$ ,  $j^D$  – dimensional values. It is seen from this figure that the kinetic and joint approaches give results with good enough agreement. At this case (pure vapour) the discrepancy between results is about 1%-3%. Also it should be noted that mass flux density obtained on the base of our kinetic solution is very closed to analogous data presented in [11].

On the next stage evaporation-condensation problem in vapour-gas mixture was solved by kinetic and joint solution method. Scheme of problem is present in Fig. 1. In the initial moment time domain between surfaces is occupied by vapour-gas mixture with numerical density  $n_a = 1.0$  (vapour) and  $n_b = 0.5$  (gas). Mixture temperature is equal 1.0 ( $T=1.0$ ). The vapour molecules emitted from interphase surfaces have Maxwell distribution function with  $T_I$ ,  $n_{aI}$ ,  $T_{II}$ ,  $n_{aII}$ . It should be noted that surfaces I and II are not penetrable for gas component, therefore the values of gas numerical densities for reflected gas molecules  $n_{bI}$  and  $n_{bII}$  are determined by non-penetration conditions. The results of solution are presented in Fig. 4. The calculations are made for case of identical mechanically molecules:  $m_a = m_b$  and  $d_a = d_b$ . As in previous problem (pure vapour) kinetic and joint solutions are agreed with good accuracy.

Solution results of the evaporation-condensation problem with the presence of non-condensable component for case of different masses and diameters of components are presented on Fig. 5-7. In this case the relation of masses and diameters component «a» to component «b» are  $m_a/m_b = 18/28$  and  $d_a/d_b = 4.6/3.7$  accordingly. Scheme of the problem is analogous a previous. Calculations are made for the cases of different numerical densities of non-condensable component ( $n_b=0.1$ ,  $n_b=0.5$ ,  $n_b=5.0$ ).

Results for case when numerical density is equal 0.1 are presented in Fig. 5. Same results for  $n_b=0.5$  and  $n_b=5.0$  are presented in Fig. 6 and Fig. 7 accordingly.

Analysis of presented figures shows that increase of gas (non-condensable) numerical density causes transformation of densities dependence on co-ordinate. If gas numerical density is small enough as in Fig. 5, then behavior of this dependence is close to corresponding curve for pure substance (see comparison Fig. 3 and Fig. 5). If gas numerical density is large enough as in Fig. 6 and Fig. 7 then densities dependence on co-ordinate is in principle other. In these evaporation-condensation processes mass flux density  $J$  with rise of gas numerical density  $n_b$  decreases. Corresponding values  $J$  for different  $n_b$  (0.1, 0.5, 5.0) are presented in Fig. 5–7 (b).

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