Joint liquid-vapor approach development at solution of different heat and mass transfer problems

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Abstract Paper is devoted to a research of heat-mass transfer processes near the boundary surface liquid-vapor taking into account interference of each phase at each other. For these purposes the approach allowing to carry out the description as a liquid and vapor phase on the basis of a uniform computing algorithm is presented. The offered approach is based on the numerical solution of the of Boltzmann kinetic equation, but at the same time the assumption of the invariance of a state (parameters) of the condensed phase isn't used. The theme of the impact of multiparticle interaction at values of macro-parameters in the vapor field and in the condensed phase is considered.

1. Introduction

It is known that at thermonuclear fusion strong non-equilibrium conditions take place. These conditions are carried out as in Tokamak installations, and at plasma inertial confinement, and in others. Two-phase systems of vapor-liquid kind are greatest interest among different heat and mass transfer processes realizations, because efficiency of boiling, evaporation and condensation is large enough.

We can consider that strict enough study of strong evaporation and condensation was begun about fifty years ago. At this time many researchers [1-7] were focused on the solution of nonlinear evaporation–condensation problems with the use of the kinetic theory of gases. Therefore the Boltzmann kinetic equation (BKE) began to be applied to the evaporation–condensation problems. The cited studies and subsequent have mainly concentrated on the solution of BKE by different methods. The Maxwell distribution function has conventionally been used to model the velocity distribution function of vapor molecules leaving the interface. Factual and empirical correlations between the interface surface temperature and saturation vapor pressure makes it possible to determine the velocity distribution function of the aforementioned molecules, which is necessary for solving BKE. However, the evaporation process is influenced by the velocity distribution of particles ejected from the interface, and the vapor parameters near the interface surface influence the interface layers of the condensed phase.

Another method for solving phase transition problems is the conjugate approach, wherein the liquid phase and the region near the interface boundary layer are described using the molecular dynamics (MD) method, following which the methods of the kinetic theory of gases are applied; finally, continuum mechanics approaches are applied for distances exceeding 10–20 mean free paths. As a research method, the MD simulation has been widely used presently. There are several known works
in which the calculation of the velocity distribution function (VDF) of molecules emitted from the interface boundary layer is performed by the MD method [8-17] and the analysis of the simulation results lead to the conclusion about the proximity of the VDF of vapor molecules “flying” from the interface to the Maxwellian distribution. However, MD application faces certain problems and difficulties. Corresponding discussion is presented in [18].

Few works have modeled liquid and gas phases within a single computational method [14, 18-21]. Correct description of evaporation and condensation can be obtained at the joint vapor-liquid problem solution just. First the authors’ attempts to develop such method were presented in the papers [22, 23]. Bellow the following step of joint approach creation is given.

In the paper [18] the possibility of the description of particles interaction in liquid as superposition of pair interactions is considered. Assumption was entered that the correlations arising at interference of a particles set at each other can be neglected owing to molecular chaos.

However the question of the impact of multiparticle interaction in the condensed phase still remains open and demands an additional research. In the presented work it is offered to consider changes of macroparameters near the boundary surface and in the condensed phase taking into account multiparticle interaction.

2. Problem statement and approach

Let’s mark in liquid group a several particles $M$ which are in close proximity from each other. Let’s assume that the marked group can be considered how a single system in which all atoms at the same time interact with all. When passing through position of equilibrium of each particle it is possible to record its velocity $(\xi_x, \xi_y, \xi_z)$. Numerous researches [17] show that, as a rule, in the condensed phase the cumulative distribution function on velocities $f(\xi)$ is close to Maxwellian.

Each particle of liquid is moving in space $(x, y, z)$, i.e. possesses three degree of freedoms. Then the system from $M$ particles will have $3M$ degree of freedoms. The condition of this system can be described by means of a vector $P$ which components are all velocities of atoms (molecules).

The interaction between all particles of the selected state group will lead to a change of system state and hence of components of vector: $P \rightarrow P'$. At this the length of the vector $|P|$ remains unchanged by virtue of the law of conservation of energy. Therefore, the process of multiparticle interaction can be interpreted as turn vector $P$ in many dimensional space: $(e_1, e_2, e_3, ..., e_j, ..., e_{3M})$ with dimension $3M$ (Figure 1). Each degree of freedom will correspond to its own axis of coordinates. For example, $e_1 \leftrightarrow \xi_x, e_2 \leftrightarrow \xi_y, e_3 \leftrightarrow \xi_z$.

![Figure 1. State vector rotation in to multidimensional space of freedom degrees](image)

To describe this transformation $P \rightarrow P'$ mathematically, it is necessary to create a turn matrix: $A$. Then the vector $P'$ is calculated as the product of the turn matrix $A$ and the original column vector $P$:

$$P' = AP$$ (1)
Turn in multidimensional space can be represented as a sequence of turns in each plane \((e_i, e_j)\). Due to molecular chaos, the angles of turn \(\alpha_{ij}\) will be determined randomly. Examples of turn matrixes \(A_{12}\) и \(A_{13}\) in the planes \((e_1, e_2)\) и \((e_1, e_3)\):

\[
A_{12} = \begin{bmatrix}
\cos \alpha_{12} & -\sin \alpha_{12} & 0 & 0 & 0 & 0 & \cdots & 0 \\
\sin \alpha_{12} & \cos \alpha_{12} & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 1
\end{bmatrix}, \quad A_{13} = \begin{bmatrix}
\cos \alpha_{13} & 0 & -\sin \alpha_{13} & 0 & 0 & 0 & \cdots & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 \\
\sin \alpha_{13} & 0 & \cos \alpha_{13} & 0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 1
\end{bmatrix}
\]

Since the turn in \(3M\)-dimensional space is considered as a sequence of turns in the planes, matrix \(A\) can be found as a sequential product of all matrixes \(A_{ij}\):

\[
A = A_{ij} \cdots A_{23} A_{13} A_{12} \cdots A_{ij}
\]

In total, the vector \(P\) can be turned in \(3M(3M - 1)/2\) planes. For example, if the system consists of 5 interacting particles, the dimension of space is 15. And the quantity of planes, in which the vector can be rotated, is equal to 105.

After finding the vector \(P'\), all components of the particle velocities after interaction become known.

The proposed approach allows us to find the distribution function directly from the computational procedure itself, without resorting to writing a complex multi-particle collision integral. Element of condensed phase consisting of from \(10^6 - 10^7\) particles is considered. The distribution function in initial time moment is assumed to be given. As a rule this function is Maxwellian. In the framework of the numerical method, continuously changing velocities are replaced by a set of values \(\{\xi_k\}\), which change with a given step \(\Delta \xi\). In this case, the distribution function also becomes discrete.

From the element of the condensed phase, we will randomly choose groups of \(m\) atoms (molecules) and consider the interactions between these particles using the approach outlined above.

Knowledge of the modified atomic velocities of atoms allows us to determine a new set of velocities for a selected group of particles. Hence, the possibility appears to define quantity of particles for a selected group of particles in the vicinity of the selected velocity point \(\xi_k\). The prime marks the velocity after interactions. By repeating the procedure of selecting groups of particles at random many times, we can construct a new distribution function.

Using the proposed approach, the evaporation-condensation process of argon was investigated. Test results were obtained. Statement of problem is shown in Figure 2. The central region, occupied by vapor, is bordered by two layers of condensate. At initial time moment vapor density \(n_0\) is equal to 33.49 kg/m³ and vapor temperature: \(T_0 = 110\) K. Temperatures of both liquid layers are equal to \(T_0\) also. In initial moment the temperature of the surface bounding the area to be studied on the left increases and becomes: \(T_1 = 120\) K. The temperature on the right remains unchanged.

Over time, the temperature of the condensate layers changes. Correspondingly conditions on the vapor condensate interfaces and evaporation intensity change also. At this the base parameters are the following: density \(n_0\) temperature \(T_0\), mean free path is calculated at \(n_0\) and \(T_0\).

In order to describe the evaporation from interface we need to know the potential energy of particle \(\varepsilon_s\), surrounded by the others atoms.
This study was carried out in [18] and [22]. To consider this fact at the solution of the evaporation-condensation problem, some approximations for potential energy were offered:

$$\varepsilon_s(T) = kT \frac{e_0}{\varepsilon} \cos \left( \frac{\pi T}{2T_k} \right)$$  \hspace{1cm} (3)

Here $T$ – liquid temperature, $k$ – Boltzmann's constant, $T_k$ – temperature close to critical temperature.

It is assumed that only those particles leave the surface of the condensed phase whose velocity satisfies the following relation:

$$\xi_x \geq \sqrt{\left( \frac{\varepsilon}{\xi_x} \right)^2 - \mu^2}$$  \hspace{1cm} (4)

where $u_s = \sqrt{2\varepsilon_s/m}$, $m$ – mass of particle (atom or molecule).

It should be noted that in the present work, the kinetic equation is solved, both in the vapor region and in the condensed phase.

For vapor this equation is the Boltzmann kinetic equation with a pair-collision integral $J$.

Kinetic equation in the liquid domain looks by analogy:

$$\frac{\partial f}{\partial t} + \xi \frac{\partial f}{\partial \xi} = Z_M$$  \hspace{1cm} (5)

The value $Z_M$ in the right part of equation (5) should be taken into account the simultaneous interaction of atoms (molecules) of the condensed phase. This value is calculated on the base of computational procedure described above. The distribution function modification is obtained as a result of multi particles interaction influence in liquid phase.

3. Results and discussion

Results of test calculations are presented in Figures 3 – 6.

Figure 3 shows the dependences of argon density on the dimensionless coordinate in the vapor phase. It is shown how the features of the interaction between particles in a liquid affect the behavior of vapor. Data shown by solid line were obtained for $M=3$, that is on the assumption about simultaneous interaction of three liquid particles. Clear rhombuses correspond calculation at $M=5$, that is for five particles interaction. The largest difference between obtained values of density is about 4%.

The blue dots in Figure 3 are results obtained on the base paper [18] algorithm. In this paper the kinetic equation is solved both in vapour and liquid region but particles interactions in this case was considered as pair interaction and collision integral is calculated as sum of these pair collisional integrals.

This approach is based on the molecular chaos assumption. The multi particles correlations are neglected in this case.
As can see from Figure 3 the differences between calculations results with taking into account of five-particles interactions \((M=5)\) and results without of multi particles correlations are maximal and equal 5.6% approximately. The data for three-particles interaction \((M=3)\) are close to results for case when multi particles correlations are not taken into account. The difference in this case not more 2%.

The temperature distributions for similar cases are presented in Figure 4. The temperatures distribution are presented inside of liquid layers and vapour region. The difference between data for \(M=5\) and without of multi particles correlation are equal 3% approximately.

The examples of velocity distribution function inside liquid are presented in Figures 7 and 8.

The velocity distribution functions for cases \(M=3\) and \(M=5\) are presented in Figure 5. As can see from these results the velocity distribution functions are close but temperature for three-particles interaction model is more than for five-particles interaction model.

The velocity distribution function for case \(M=3\) is marked by solid line in Figure 6. The Maxwell velocity distribution function of molecules is presented also for comparison. This function is marked on this figure by dots.
As can see clear the velocity distribution function inside condensed phase is close to Maxwell function, as expected.

4. Conclusion

An approach of joint solution of heat and mass transfer problems solution into liquid and vapour region is presented. The main advantage of presented approach is the possibility of calculation the heat and mass transfer processes occurs both into liquid and vapor region with taken into account of multi-particle interaction inside liquid phase in non-steady statement (on each time step).

Proposed method was applied to investigation of argon flow between two liquid layers. Wherein the heat transfer processes inside condensed phases processes were taken into account.

The macro parameters distributions along coordinate for different time moments are presented.

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