



Non-equilibrium phenomena on the gas-liquid interface

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Key words: Evaporation, condensation, Knudsen layer, rarefaction parameter

Abstract

Evaporation and condensation processes between two parallel condensed phases are simulated using the kinetic models (S-model and BGK model). The compressible Navier-Stokes equations subjected the temperature and pressure jump conditions on the liquid-vapor interphase are also solved numerically. The results obtained from different model are compared. It was found that the Navier-Stokes model subjected to the jumps conditions provide the results close to the kinetic simulations results.

1 Introduction

Evaporation and condensation phenomena are interesting from the fundamental point of view [?], they are also largely present in various industrial applications. The correct and detailed description of these physical processes requires the application of the kinetic theory based approaches [1], [8]. However, the implementation of the kinetic approaches for the practical problems is not so easy. This is why it is interesting to use the classical Navier-Stokes equations with the temperature and pressure jumps boundary conditions [5] to simulate the evaporation-condensation problems.

The main objective of this study is the development of the mathematical model to simulate the behavior of the vapor phase at the liquid-gas interface.

First the S-model [7] kinetic approach is used to simulate the evaporation-condensation phenomena appearing between two parallel plates maintained at different temperatures. Then, these kinetic results are compared with that obtained from the Navier-Stokes equations subjected to the special temperature and pressure jumps boundary conditions [5]. These conditions were derived to take into account the non-equilibrium behaviors of a gas during the evaporation and condensation on the vapor-liquid interface. The comparison between two solutions allows us to determine the domain of the applicability of the Navier-Stokes equations with the jump conditions.

1.1 Problem statement

We consider two parallel plane gas - liquid interfaces at rest, maintained at temperature T_1 and T_2 , ($T_2 > T_1$) at the bottom ($y = 0$) and top ($y = H$) interfaces, respectively. We investigate the behavior of the steady gas flows caused by evaporation and condensation on the condensed phases on the basis of kinetic theory. Let p_1 be the saturation gas pressure at temperature T_1 and p_2 that at temperature T_2 . The problem is characterized by the parameters p_2/p_1 and T_2/T_1 and by the rarefaction parameter δ . The saturation gas pressure is a function of the saturation gas temperature given by the Clausius-Clapeyron equation [4].

The S-model kinetic equation is written as

$$\frac{\partial f}{\partial t} + \mathbf{v} \frac{\partial f}{\partial \mathbf{r}} = Q(f, f), \quad (1)$$

where $f(t, \mathbf{r}, \mathbf{v})$ is the velocity distribution function of gas molecules, \mathbf{v} is the molecular velocity vector, \mathbf{r} is the position vector, t is a time. In the frame of S-model kinetic equation the collision term $Q(f, f)$ has the form

$$Q(f, f) = \nu(f^S - f), \quad (2)$$

where ν is the collision frequency, f^S is an equilibrium distribution function defined by

$$f^S(\mathbf{r}, \mathbf{v}, t) = f^M \left[1 + \frac{2m(\mathbf{v} - \mathbf{u})\mathbf{q}}{15n(\mathbf{r})(kT(\mathbf{r}))^2} \left(\frac{m(\mathbf{v} - \mathbf{u})^2}{2kT(\mathbf{r})} - \frac{5}{2} \right) \right], \quad (3)$$

here $T(\mathbf{r})$ is a gas temperature, $n(\mathbf{r})$ is a gas number density, \mathbf{u} is a bulk velocity, \mathbf{q} is a heat flux, m is a mass of gas molecule, k is the Boltzmann constant.

The boundary conditions for the plane vapor-liquid interface can be written as

$$f^+ = (\alpha n_i + (1 - \alpha)n_{wi})f_w^i, \quad i = 1, 2, \quad (4)$$

$$f_w^i(\mathbf{v}) = \left(\frac{m}{2\pi kT_i} \right)^{3/2} \exp(-m\mathbf{v}^2/(2kT_i)), \quad (5)$$

n_i is the number density of the saturated vapor near the plane interface, it can be calculated from the equation of state using the values of the saturated pressure at the saturated temperature as $n_i = p_i/(kT_i)$. α is the evaporation and condensation coefficient, here we supposed that both coefficients are equal. The number density n_{wi} ($i = 1, 2$) can be found from the relation:

$$n_{wi} \sqrt{\frac{kT_i}{2\pi m}} = \int_{\mathbf{nv} < 0} v_y f^- d\mathbf{v}. \quad i = 1, 2. \quad (6)$$

If the function f is known the macroscopic parameters are defined:

$$n(\mathbf{r}, t) = \int f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v}, \quad (7)$$

$$T(\mathbf{r}, t) = \frac{m}{3kn} \int f(\mathbf{r}, \mathbf{v}, t) V^2 d\mathbf{v}, \quad (8)$$

$$\mathbf{q}(\mathbf{r}, t) = \frac{m}{2} \int f(\mathbf{r}, \mathbf{v}, t) V^2 \mathbf{V} d\mathbf{v}, \quad (9)$$

here $\mathbf{V} = \mathbf{v} - \mathbf{u}$. The mass flow rate can be calculated as

$$J_N = \int v_y f(\mathbf{r}, \mathbf{v}, t) d\mathbf{v}. \quad (10)$$

The distance H between the two interfaces is taken as the characteristic dimension of the problem. The Knudsen number and the rarefaction parameter are defined as following:

$$Kn = \frac{\ell}{H}, \quad \delta = \frac{1}{Kn}, \quad \ell = \frac{\mu_1 \sqrt{2\mathcal{R}T_1}}{p_1}, \quad (11)$$

here ℓ is the equivalent mean free path, μ_1 is the dynamic viscosity of the vapor phase and $\sqrt{2\mathcal{R}T_1}$ is the most probable molecular speed, both at the temperature T_1 , \mathcal{R} is the specific gas constant.

2 Results

The evaporation-condensation between two condensed planes is simulated by two kinetic models (BGK and S-model) and by using the compressible Navier-Stokes equations with the temperature and pressures jumps boundary conditions [5], [3] for several sets of the rarefaction parameter (Knudsen number), temperature and pressure ratios.

As an example the evaporation and condensation of Argon is considered between two parallel condensed phases.

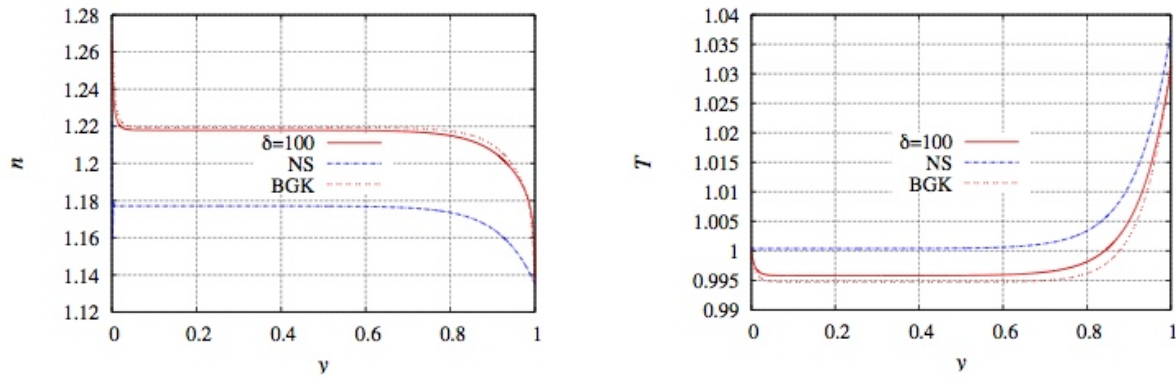


Figure 1: The number density (left) and temperature (right) profiles.

The temperature ratio is equal to $T_2/T_1 = 1.036$, $p_2/p_1 = 1.459$. The rarefaction parameter δ is equal to 100 which corresponds to the slip flow regime. The comparison between the results obtained with the kinetic models (S-model and BGK model) and the Navier-Stokes equations with the temperature and pressure jumps boundary conditions are provided on Figure 1. Relatively good agreement is found between all three approaches.

The inverse temperature gradient phenomenon [1] can be observed: the vapor temperature near the colder (condensed phase) is hotter as that near the hotter phase.

Further simulations are needed to find the conditions of the applicability of the Navier-Stokes equations with the jumps boundary conditions.

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