MIGRATE DRAFT 156588

Numerical simulation of evaporation and condensation phenomena around a small condensed phase droplet

V.B. Leite[A 1], **D. Kalempa**[A 2], and **I. Graur**[B 3]

[A]Department of Basic and Environmental Sciencies, Lorena School of Engineering, São Paulo University, Lorena,Brazil
[B]Aix-Marseille Université, CNRS, IUSTI UMR 7343, Marseille,France
vinicius.bl@alunos.eel.usp.br[1], kalempa@usp.br[2], irina.martin@univ-amu.fr[3]

Key words

Aerosols, Boltzmann equation, rarefied gas, evaporation/condensation at surface.

Abstract

Despite of the several decades of researches regarding evaporation and condensation phenomena on surfaces, these phenomena are not yet well understood [1]. The continuum mechanics equations, the Navier-Stokes (NS) equations, widely used in engineering areas, are not always valid to describe correctly the non-equilibrium phenomena such as evaporation and condensation in a gaseous media. These equations are valid only when the Knudsen number, Kn, defined as the ratio between the molecular mean free path and the characteristic dimension of the gaseous system, is small enough, *i.e.* the gas rarefaction degree is sufficiently small to consider a gaseous medium as a continuum. But even when the Knudsen number is small, a thin layer (the Knudsen layer) exists on the interface between the liquid and gaseous phases. Therefore, the implementation of the methods based on the kinetic theory of gases [2, 4] are indispensable to describe correctly the phenomena occurring during evaporation and condensation.

The present work aims the numerical simulation of the condensation and evaporation phenomena at the surface of a spherical droplet of the condensed vapour by using the numerical solution of the linearized kinetic equation proposed by Shakhov [5].

We consider a gas around a spherical droplet, of radius R_0, of its condensed phase at constant temperature T_w. Far from the droplet the gas is at an equilibrium state (pressure p_0 and temperature T_0). We investigate the steady evaporation from (or condensation onto) the spherical condensed phase under the following assumptions:

(i) The gas flow around the sphere is described by the model proposed by Shakhov [5] for the linearized Boltzmann equation.

(ii) The fraction α of the molecules emitted from the particle surface is evaporated in an equilibrium manner while the fraction $(1-\alpha)$ is reflected from the surface in accordance with a diffusive law with total temperature accommodation. The velocities of the reflected molecules are distributed according to the Maxwellian law.

(iii) The ratios $\nu_s = |n_s - n_0|/n_0$ and $\tau_s = |T_s - T_0|/T_0$ are assumed to be small enough to allow the linearization of the kinetic equation and of the boundary conditions around the equilibrium state at rest, far from the sphere, with the number density n_0 and temperature T_0. n_s and T_s are the saturated number density and temperature of the condensed phase.

The linearized kinetic equation with the boundary conditions is solved by the Discrete Velocity Method (DVM). The bulk velocity of the gas evaporated from the surface can be found as following: $2u_r = G_\nu \nu_s + G_\tau \tau_s$, where G_ν and G_τ are the quantities related to the bulk velocity of the gas for the density deviation and temperature deviation, respectively. These quantities depend only on Kn and the evaporation-condensation coefficient α. The numerical results for the G_ν and G_τ coefficients are presented in Tables 1 and 2 for several values of the rarefaction parameter δ. The comparison with the results presented in Refs. [3, 6] shows a good agreement.

Table 1: The values of G_υ depending on the rarefaction parameter δ and evaporation coefficient α

				α			
δ	0.1	0.2	0.4	0.5	0.7	0.8	1.0
0.01	0.0562	0.112	0.225	0.281	0.394	0.450	0.563
0.05	0.0562	0.113	0.226	0.283	0.397	0.454	0.569
0.1	0.0563	0.113	0.227	0.284	0.400	0.458	0.576
0.3	0.0565	0.114	0.230	0.290	0.411	0.473	0.600
0.5	0.0567	0.114	0.233	0.295	0.421	0.486	0.620
0.7	0.0568	0.115	0.236	0.298	0.429	0.496	0.637
1.0	0.0570	0.116	0.239	0.303	0.439	0.510	0.659
2.0	0.0573	0.117	0.245	0.314	0.462	0.541	0.713

Table 2: The values of G_τ depending on the rarefaction parameter δ and evaporation coefficient α

				α			
δ	0.1	0.2	0.4	0.5	0.7	0.8	1.0
0.01	0.0282	0.0563	0.113	0.141	0.197	0.226	0.282
0.05	0.0284	0.0569	0.114	0.143	0.200	0.229	0.287
0.1	0.0287	0.0576	0.116	0.145	0.204	0.233	0.293
0.3	0.0300	0.0605	0.122	0.154	0.219	0.251	0.318
0.5	0.0312	0.0631	0.129	0.163	0.233	0.269	0.344
0.7	0.0323	0.0655	0.135	0.171	0.246	0.286	0.368
1.0	0.0337	0.0686	0.143	0.182	0.265	0.309	0.403
2.0	0.0370	0.0761	0.162	0.209	0.313	0.371	0.499

Acknowledgement

The authors would like to acknowledge the financial support provided by FAPESP (Fundação de Amparo à Pesquisa do Estado de São Paulo, Brazil), project number 2016/09118/2.

References

[1] Bird, G. A., Molecular Gas Dynamic and the Direct Simulation of Gas Flows, *Oxford University Press*, Oxford, 1994.

[2] Cercignani, C., The Boltzmann equation and its application, *Springer-Verlag*, New York, 1988.

[3] Chernyak, V., The Kinetic Theory of Droplet Evaporation, *J. Aerosol Sci., Vol. 26, No. 6, pp. 873-885*, 1995.

[4] Kennard, E. H., Kinetic theory of gases, *McGraw-Hill Book Companhu Inc.*, 1938.

[5] Shakov, E. M., Generalization of the Krook Kinetic Equation, *Fluid Dynamics*, 1968.

[6] Takata, S., Sone, Y., Lhuillier, D. and Wakabayashi, M., Evaporation from or Condensation onto a Sphere: Numerical Analysis of the Boltzmann Equation for Hard-Sphere Molecules, *Computers Math. Applic. Vol. 35, No. 1/2, pp. 193-214*, 1998.