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COMPARISON OF NUMERICAL RESULTS OF MOLECULAR DYNAMICS SIMULATIONS AND S-MODEL KINETIC EQUATIONS FOR EVAPORATION AND CONDENSATION OF ARGON

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KEY WORDS

Molecular dynamics, S-model kinetic equation, Evaporation, Condensation, Liquid-Vapor interface, Rarefaction parameter

SHORT SUMMARY

The applicability of the S-model kinetic equation for simulation of evaporation and condensation phenomena is investigated by comparing its results for Argon with those of Molecular Dynamics (MD). The steady-state evaporation and condensation between two liquid Argon layers, kept at different but constant temperatures, is simulated. The temperature ratio between the hot/cold Argon layers is fixed at $T_1/T_2 = 1.045$ and the rarefaction parameter is equal to $\delta = 7.9$, which corresponds to the beginning of transitional flow regime. The macroscopic profiles of temperature and heat flux in vapor between the liquid layers are depicted. Both methods predict an inverted temperature profile. The agreement between the methods depends on the evaporation/condensation coefficients and the temperature at the liquid boundaries. Therefore, it is important to obtain the evaporation/condensation coefficients and the positions of the liquid boundaries accurately.

EXTENDED ABSTRACT

The development of microscale cooling systems becomes important due to the increasing heat transfer density within electrical devices. These systems need to dissipate higher heat fluxes using less energy compared to existing cooling systems if the next generation of high-power electronic devices are to be enabled. This can be achieved by a new generation of two phase flow evaporative systems. Such device contains a nanopores structure through which the liquid evaporates and the latent heat of vaporization is the dominant mode of heat transfer. Therefore, the understanding of evaporation/condensation process and corresponding vapor flow behaviors in and around these nano-structures is important for the development of these cooling systems. The applicability of the S-model kinetic equation to describe these processes will be investigated by comparing its results with those of the MD simulations. The order of the pressure and temperature jumps at the liquid-vapor interface, provided by both approaches will be also analyzed.

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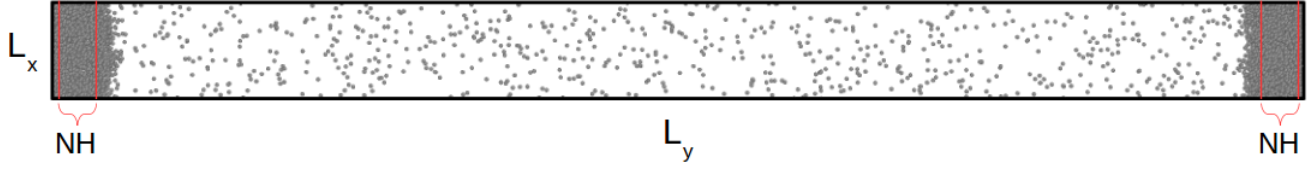


Figure 1: Numerical simulation domain for molecular dynamics with a Nose-Hoover (NH) thermostat applied to a part of the liquid phase.

The numerical set-up for this comparison consists of a steady-state heat transfer through Argon vapor between its two liquid layers. The ratio of the liquid temperatures is $T_1/T_2 = 1.045$ with $T_1 = 104.5K$ and $T_2 = 100K$. The corresponding saturation pressures are $p_{sat}(T_1) = 0.4777394 \cdot 10^6$ Pa and $p_{sat}(T_2) = 0.325021 \cdot 10^6$ Pa. The vapor rarefaction parameter is defined as,

$$\delta = \frac{L_v}{\lambda} \quad \text{with} \quad \lambda = \frac{1}{\sqrt{2}\pi n \sigma^2}, \quad n = \frac{p_{sat}(T_2)}{k_B \cdot T_2} \quad (1)$$

where λ denotes the molecular mean free path, L_v is the length of the vapor phase, n is the number density obtained from the ideal gas law, σ is the molecular diameter, $\sigma = 0.34$ nm for Argon, and k_B is the Boltzmann constant. Substitution of the given numbers into relations (1) implies that $n = 0.23454 \cdot 10^{27} \text{m}^{-3}$, $\lambda = 8.3 \cdot 10^{-9}$ m and the rarefaction parameter $\delta = 7.9$.

In Fig.1, the numerical simulation domain for MD is depicted with dimensions of: $L_x = L_z = 5.75$ nm and $L_y = 75.0$ nm, and periodic boundary conditions are applied in each direction. The Lennard-Jones 12-6 potential is used to calculate the intermolecular forces between the Argon particles with parameters: $\epsilon = 0.24036$ Kcal/mol and cut-off distance $r_c = 2.55$ nm (7.5σ). A Nose-Hoover thermostat is applied to the regions ($\Delta y = 2.0$ nm) indicated by NH in Fig.1. The distance between the vapor boundary and the thermostat is approximately 7σ on both sides. The liquid and vapor boundaries are determined by following the procedure given by Meland [1]. Because the thickness of the liquid layers at the evaporation/condensation sides are decreasing/increasing, a steady-state is achieved by shifting the atoms in y -direction during the simulation [1]. Therefore, the average number of atoms in the liquid on both sides remains equal. The results are obtained by averaging from 1 ns to 20 ns, in which the time step for the simulation was $\Delta t = 4$ fs.

The steady-state dimensionless form [4] of the S-model kinetic equation is defined as,

$$\mathbf{c} \frac{\partial f(y, \mathbf{c})}{\partial y} = \delta n \sqrt{T} (f^S - f) \quad (2)$$

where, $f(y, \mathbf{c})$ is the one particle molecular velocity distribution function, \mathbf{c} is the molecular velocity vector, y is the distance between the liquid layers, see Fig.1, and f^S the equilibrium distribution function [4]. The S-model kinetic equation is solved by the discrete velocity method in one-dimensional in the physical space and two dimensional in the molecular velocity space formulation. When the numerical values of the distribution function f are obtained the macroscopic profiles like temperature, pressure and number density are calculated by its integration over the molecular velocities.

At the liquid-vapor interface, the following boundary conditions are used. We assume that only one part β of the incident molecules evaporates immediately and $(1 - \beta)$ part reflects from the surface diffusively. Therefore the dimensionless boundary conditions for the distribution function of

the reflected molecules at the liquid-vapor interfaces can be written as,

$$\begin{aligned}
 y &= 0, & c_y > 0 \\
 f &= (\beta n_{s_1} + (1 - \beta)n_{r_1})f_1^M, & f_1^M &= \frac{1}{\pi^{3/2}} \frac{p_1}{p_2} \left(\frac{T_2}{T_1}\right)^{5/2} \exp\left(-\frac{T_2}{T_1}c^2\right) \\
 y &= 1, & c_y < 0 \\
 f &= (\beta n_{s_2} + (1 - \beta)n_{r_2})f_2^M, & f_2^M &= \frac{1}{\pi^{3/2}} \exp(-c^2)
 \end{aligned} \tag{3}$$

Here n_{s_i} , $i = 1, 2$ is the number density of the saturation vapor near each interface, calculated from the equation of state using the values of the saturation temperature and corresponding saturation pressure. The number density n_{r_i} , $i = 1, 2$, can be calculated from the impermeability condition on the corresponding interface,

$$n_{r_1} = -2\sqrt{\pi} \sqrt{\frac{T_1}{T_2}} \int_{c_y < 0} c_y f d\mathbf{c}, \quad n_{r_2} = 2\sqrt{\pi} \int_{c_y > 0} c_y f d\mathbf{c} \tag{4}$$

In present comparison the case of the complete evaporation, $\beta = 1$, is considered.

Results and Conclusions

The temperature and heat flux profiles are calculated using the peculiar velocity $\mathbf{V} = \mathbf{c} - \mathbf{u}$, with \mathbf{u} the vapor bulk velocity. In Fig.2(a), the temperature profile of the vapor phase is depicted for MD and the S-model numerical results. Both methods predict an inverted temperature gradient profile which occurs when $\Delta P/\Delta T > 4.7723$ [2,3] which is the case here. The important temperature jump is found near both liquid phases. The vapor temperature near the hotter phase $T_v/T_2 \sim 1.005$, $y = 0$, is lower than the temperature of the hotter liquid phase, $T_1/T_2 = 1.045$. Contrarily, near the colder liquid phase, $y = 1$, the vapor temperature, $T_v/T_2 \sim 1.035$, is higher than that of the liquid phase, $T_2/T_2 = 1$. The heat flux profiles are shown in Fig.2(b). The results coincide near $y = 0$ for both temperature ratios, but deviates from the MD results towards $y = 1$ when using the smaller temperature ratio, $T_1/T_2 = 1.045$.

It is concluded that the position of the liquid boundaries from which the liquid temperature is extracted has a large influence on the results of the S-model. A small change of the position of the liquid boundary at the evaporation side (resulting in a temperature shift of +0.3K), improves the agreement between both methods considerably (Fig.2, black lines). Furthermore, the evaporation/condensation coefficients have a large influence as well (not depicted). Therefore, it is important to obtain the evaporation/condensation coefficients and the position of the liquid boundaries in an accurate and robust way.

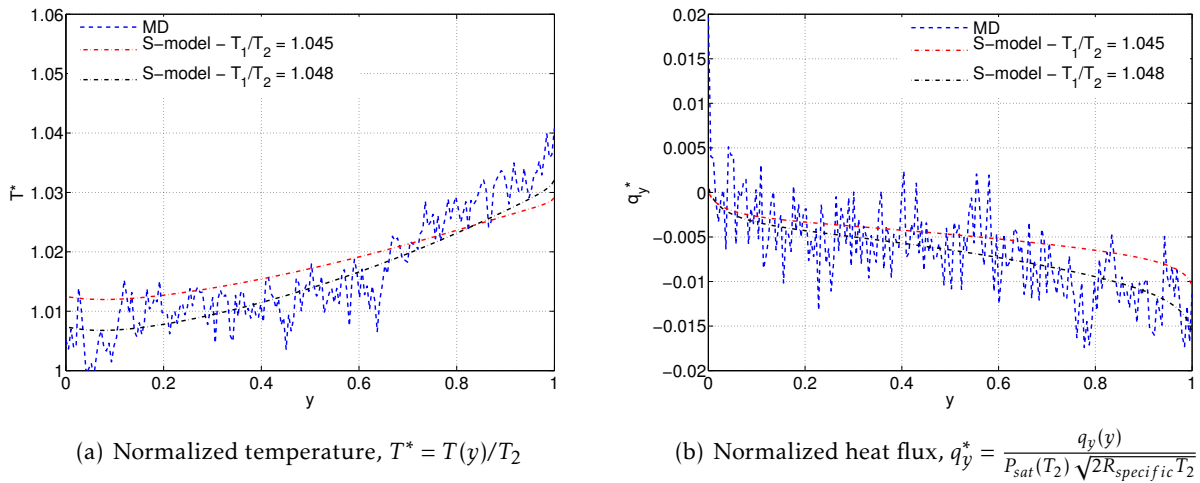


Figure 2: Temperature and heat flux profiles for MD and the S-model

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