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THE POSITION OF THE LIQUID AND VAPOR BOUNDARIES AND ITS INFLUENCE ON THE EVAPORATION/CONDENSATION COEFFICIENTS

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KEY WORDS

Molecular dynamics, S-model kinetic equation, Evaporation & Condensation coefficient, Liquid-Vapor interface, Liquid boundary, Vapor boundary, Kinetic boundary conditions

ABSTRACT

Introduction

Thermal management of electronics has become important due to the miniaturization of electronic devices during the last decades. This has increased the heat transfer density within those devices and need to be compensated by the development of an advanced microscale cooling system[1]. A potential solution is the two-phase flow evaporative cooling system, see fig.1. Within these systems, a liquid evaporates through a nanopores membrane with the latent heat of vaporization to be the dominant mode of heat transfer. The nanopores geometry generates the requisite capillary pressure to drive the liquid flow to the heat source.

This system consist of multiple flow regimes. The heat transfer within the ridges and liquid can be considered in the continuum regime whereas the evaporation from the nanopores membrane should be considered in the transition/free molecular regime. Therefore, a multiscale modeling approach has to be developed. The evaporation process and its vapor flow from the nanopores will be described by kinetic models / DSMC and Molecular Dynamics (MD) simulations. The first approach in construction this multiscale modeling setup is the validation of the kinetic model, which is the S-model kinetic equation [2] and its kinetic boundary conditions (KBC).

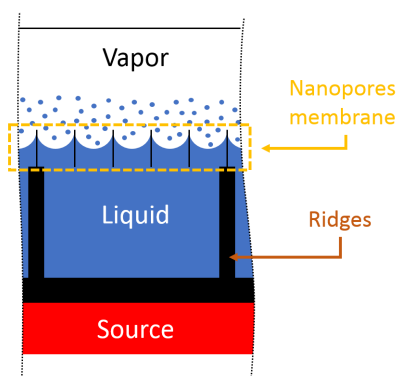


Figure 1: Simplified schematic of evaporative cooling system (not to scale).

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Liquid and vapor boundaries

The vapor phase in the vicinity of the liquid-vapor interface during net evaporation is a non-equilibrium region. KBC based on the molecular velocity distribution functions are able to describe the vapor flow within this region [3]. They include the so-called evaporation (α_e) and condensation (α_c) coefficients defined as,

$$\alpha_e = \frac{\langle J_{evap} \rangle}{\langle J_{out} \rangle}, \quad \alpha_c = \frac{\langle J_{cond} \rangle}{\langle J_{coll} \rangle} \quad (1)$$

with $\langle J_{...} \rangle$ the time-averaged mass fluxes of the evaporating, condensing, reflecting and colliding atoms. These fluxes are calculated from MD simulations by defining a liquid and vapor boundary, see fig.2.

Different methods have been developed to determine the position of these boundaries. Meland[4], defined the vapor boundary as the position "near the liquid" where $|p - p_{SRK}|$ is greater than the maximum of $|p - p_{SRK}|$ in the vapor phase. With SRK the Soave-Redlich-Kwong (SRK) equation of state and p the vapor pressure. For the liquid boundary he used the density-gradient thickness. Gu *et al.*[5], used a microscopic approach by counting the interacting molecular partners $\overline{N'_i(t)}$ per molecule in a specially constructed volume, V' about each molecule in the simulation. The liquid and vapor regions are defined by $\overline{N'_i(t)} \geq C_l$ and $\overline{N'_i(t)} \leq C_v$ respectively. The values of C_l and C_v are obtained from separate MD simulations consisting of either a pure liquid or vapor phase.

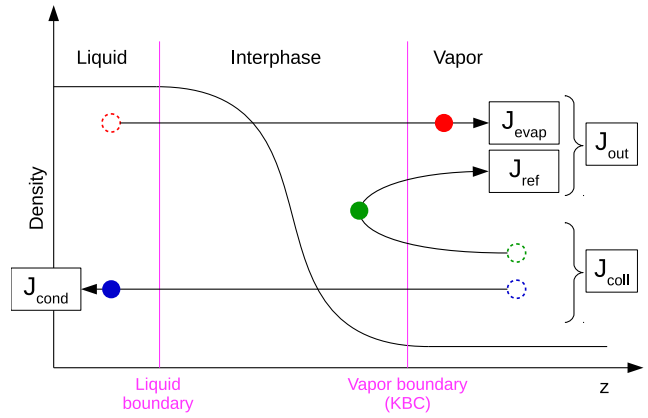


Figure 2: Schematic of the liquid-vapor interface and the evaporation, condensation and reflecting molecules

Once the boundary positions are determined, the atoms will be labeled according to their initial phase (liquid or vapor). The mass fluxes are calculated by tracking the particles during the simulation[4]. Atoms crossing the vapor boundary with their initial state in the liquid phase are counted as evaporated (red circles in fig.2). Whereas atoms crossing the liquid boundary which were initially in the vapor phase will be counted as condensed (blue circles in fig.2). The outgoing and colliding fluxes consist from all atoms crossing the vapor boundary with $v_z > 0$ and $v_z < 0$ respectively, see fig.2.

Because each method (Meland, Gu,..) defines the liquid and vapor boundary positions in a different way, the corresponding liquid temperatures and evaporation/condensation coefficients will differentiate between the methods. Therefore we will focus on how to determine these boundaries purely by MD simulations.

Table 1: Properties for the simulation of Argon

Molecular mass m [kg]	Length σ [m]	Interaction energy ϵ [Kcal/mol]	Cut-off distance r_c [nm]	Time step Δt [fs]
6.64×10^{-26}	3.4×10^{-10}	0.24036	2.04	4

The numerical domain of the MD simulation for extracting the evaporation and condensation coefficients is depicted in Fig.3. 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 using the parameters given in Table 1. At T_1 and T_2 a Nosé-Hoover thermostat is applied. A steady-state simulation is obtained by shifting the atoms in z -direction during the simulation [4]. The macroscopic properties are obtained by time-averaging from 1 ns to 20 ns.

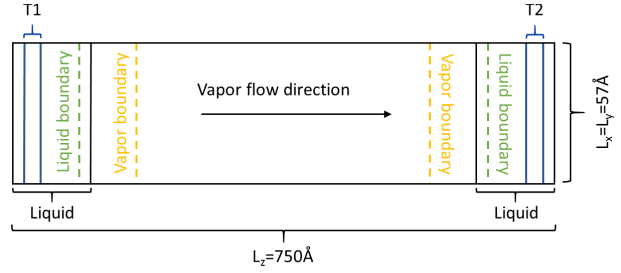


Figure 3: Schematic of the MD simulation domain.

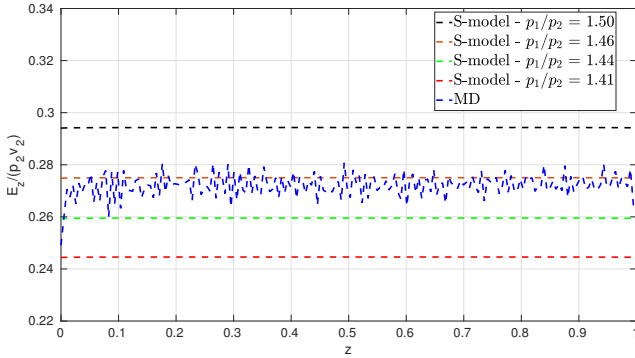


Figure 4: Numerical results of the dimensionless energy flux computed from MD and S-model equation[6]. The S-model result is computed for different saturation vapor pressures ratios using the Antoine equation.

During a previous study[6], a large discrepancy was observed in the energy flux between the numerical results of MD and the S-model equation, fig.4. The method of Meland[4] was used to determine the positions of the liquid and vapor boundary. It was observed that a small change of the pressure ratio (p_1/p_2) which corresponds to a small change of the liquid temperature ratio (T_1/T_2), has a large influence on the agreement between the MD and S-model results (see figure 4). Therefore, the following questions are defined,

- Are the existing methods robust and accurate enough in determining the liquid and vapor boundaries or is it necessary to develop a new method?
- How are the evaporation and condensation coefficients influenced by the position of both boundaries for (non)-equilibrium simulations?

Results

A non-equilibrium MD simulation has been performed with $T_1 = 104.5K$ and $T_2 = 100K$. The method of Meland[4] has been applied to the density profile to determine the liquid and vapor boundaries. While keeping the liquid boundary position fixed ($z = 29.716\text{Å}$), the vapor boundary has been shifted in the range from $z = 30\text{Å}$ to 130Å in order to see its dependence on the evaporation and condensation coefficients. The results are shown in figure 5. The maximum values of the coefficients within the vapor phase are $\alpha_e = 0.859$ and $\alpha_c = 0.810$ at $z \approx 45\text{Å}$ and decreasing afterwards.

Next, the same procedure has been repeated with the liquid boundary shifted to $z = 19.716\text{Å}$. The maximum values of the evaporation and condensation coefficients decreased to $\alpha_e = 0.762$ and $\alpha_c = 0.674$. This is showing the importance of the choice of the position of the liquid boundary.

In the case the liquid-vapor is in equilibrium or weak non-equilibrium, the outgoing mass flux J_{out}^* can be written as [7,8],

$$J_{out}^* = \rho^* \sqrt{\frac{R_{spec} T_L}{2\pi}} \quad (2)$$

with ρ^* the saturation vapor density and T_L the temperature at the liquid boundary.



An equilibrium MD simulation has been performed at $T_1 = T_2 = 100K$ and the discrepancy between the MD particle tracking and the theoretical expression (2) for the outgoing mass flux $\langle J_{out} \rangle$ investigated. Positioning the liquid and vapor boundary (Meland) at $z = 29.716\text{\AA}$ and $z = 114.20\text{\AA}$, the MD results are $\alpha_e = \alpha_c = 0.681$, whereas using the theoretical expression (2) for $\langle J_{out} \rangle$, $\alpha_e^* = \alpha_c^* = 0.587$. Hence, the discrepancy can be a consequence of the liquid and vapor boundary position.

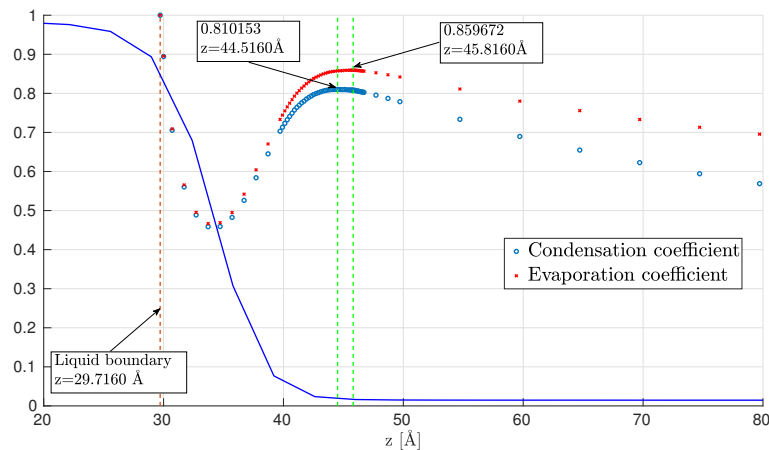


Figure 5: Evaporation and condensation coefficients for different positions of the vapor boundary at the net evaporation side. Normalized density profile (blue solid line)

Conclusions

- The position of the liquid and vapor boundary has a large influence on the evaporation and condensation coefficients
- In the case of equilibrium, J_{out}^* (2) overestimate the outgoing mass flux. Although, shifting both liquid and vapor boundary can provide better agreement.
- Further investigation is needed in the development and comparison of existing methods for determining the liquid and vapor boundary

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