



Prediction of thermal conductance at liquid-gas interfaces using molecular dynamics simulations

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ABSTRACT

Using molecular dynamics (MD) simulations and theoretical calculations, we study heat transfer across liquid-gas interfaces within a planar heat pipe. To determine the thermal conductance (Kapitza conductance), G_K , at the interface, two heat transfer mechanisms, namely, conduction and evaporation/condensation are considered. In the case of interfacial heat conduction, gas molecules, particularly non-condensable gas molecules, exchange heat with liquid surfaces through gas-liquid collisions, and the theoretical expression for G_K is derived from the kinetic theory of gases. For interfacial heat transfer by evaporation or condensation, the theoretical expression for G_K is derived from the Schrage relationships. To assess the accuracies of the theoretical expressions for G_K , we compare these theoretical predictions to the G_K obtained directly from MD simulations. For all cases studied, the theoretical predictions agree with the MD simulation results very well. If the density of non-condensable gas in the heat pipe is much higher than that of the working fluid in the gas phase, we find that the interfacial heat conduction could contribute significantly to the total heat flux across the liquid-gas interfaces. The effect of G_K at liquid-gas interfaces on the overall heat transfer efficiency in a planar heat pipe is discussed.

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1. Introduction

Due to the existence of interfacial thermal resistance (Kapitza resistance) [1] R_K , heat flow across material interfaces can result in a discontinuous temperature drop at the interface. Since the thermal resistance at the interface between helium and a solid was first reported by Kapitza [2], R_K at a variety of solid-solid, solid-liquid, and solid-gas interfaces have been extensively studied by experiments, theoretical calculations, and numerical simulations [3–5]. Similarly, heat flow across a liquid-gas interface can also result in a temperature drop at the interface [6,7]. The ability to accurately predict R_K (or its inverse G_K) at liquid-gas interfaces is important for the thermal analysis of various types of heat pipes [8] and evaporation of liquid droplets [6]. For example, heat transfer efficiency in micro/nanoscale heat pipes is strongly limited by the R_K at liquid-gas interfaces [8]. A good understanding of heat transfer mechanisms at liquid-gas interfaces can help design heat pipes with optimized cooling performance.

In spite of its importance, the studies on R_K at liquid-gas interfaces are rare. One of the difficulties in the determination of R_K at liquid-gas interfaces is that the heat transfer across a liquid-gas interface often accompanies evaporation or condensation

processes. Therefore, two heat transfer mechanisms, namely, conduction and evaporation/condensation should be considered in the analysis of heat transfer across liquid-gas interfaces. For heat transfer across solid-solid, solid-liquid, and solid-gas interfaces, only heat conduction needs to be considered in most cases.

The heat conduction at liquid-gas interfaces is due to collisions between gas molecules and liquid surfaces. Such a heat transfer mechanism is similar to that at solid-gas interfaces. The R_K at solid-gas interfaces is well predicted by theoretical expressions derived from the kinetic theory of gases [9–12]. Hence, we will employ these theoretical expressions to study conduction resistance at liquid-gas interfaces. Evaporation and condensation are processes by which a fluid transitions between its liquid state and its gas state at the liquid-gas interface. Recent molecular dynamics (MD) simulation results [8,13,14] show that the Schrage relationships [15,16] give an excellent prediction of the evaporation/condensation rates. Therefore, we will use theoretical expressions derived from the Schrage relationships to predict the evaporation/condensation thermal resistance at liquid-gas interfaces. Evaporation and condensation often occur when there is a non-condensable gas (NCG) in the gas phase, e.g. water evaporation/condensation in air. In this case, thermal energy can be transferred across the liquid-gas interface by both conduction (i.e., collisions between NCG molecules and liquid surfaces) and evaporation/condensation (i.e., liquid-vapor phase change of the

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working fluid at the interface). In our previous MD studies [8,13], the heat transfer by conduction at the liquid-gas interface is neglected in the thermal analysis of the steady-state evaporation and condensation processes. In this work we take into account both conduction resistance and evaporation/condensation resistance at the liquid-gas interface, and investigate the contribution of conduction to the overall heat flow during evaporation/condensation processes.

In the next section, we will introduce the theory for thermal transport across a liquid-gas interface and the theoretical expressions for conduction resistance and evaporation/condensation resistance at liquid-gas interfaces. To assess the accuracies of the theoretical expressions, we will compare these theoretical predictions with the R_K obtained directly from MD simulations, which require no assumptions concerning the heat transfer mechanism at the liquid-gas interface. In Section 3 we describe the MD model for the study of heat transfer across liquid-gas interfaces, and the basic properties of the model fluid. In Section 4 we present MD simulation results, and discuss how the R_K at liquid-gas interfaces affect the heat transfer efficiency in planar heat pipes. Finally, we close with a summary and conclusions.

2. Theory

The interfacial thermal conductance (or Kapitza conductance), G_K , is defined as the ratio of heat flux across the interface to the temperature drop, ΔT , at the interface [1]:

$$G_K = q/\Delta T. \quad (1)$$

where the subscript K stands for Kapitza. Depending on the heat transfer mechanism, different theoretical expressions can be used to predict G_K at a liquid-gas interface.

2.1. Interfacial heat transfer by conduction

In the case of heat conduction across liquid-gas interfaces, there is no net mass flux at the interface, and gas molecules exchange thermal energies with liquid surfaces through gas-liquid collisions/interactions. The kinetic theory of gases predicts that the conduction resistance, $R_{K,cond}$, at liquid-gas interfaces is determined by the frequency of collisions between gas molecules and the liquid surface, and the efficiency of the thermal energy

exchange during the liquid-gas collision process [9]. For incident gas molecules with an average temperature, T_g , and a density, ρ_g , the liquid-gas collision rate per area, N_g , is given by [9]:

$$N_g = \rho_g v_n = \rho_g \sqrt{RT_g/2\pi M_g}, \quad (2)$$

where v_n is the average normal velocity of incident gas molecules, M_g is the molar mass of gas molecules, and R is the gas constant. The heat exchange efficiency at a liquid-gas interface can be quantified by the thermal accommodation coefficient (TAC). For monoatomic gases, the TAC, α_T , is defined by [17]:

$$\alpha_T = \frac{T_r - T_i}{T_L - T_i}, \quad (3)$$

where T_i and T_r are the temperatures of incident and reflected gas molecules, respectively, and T_L is the liquid surface temperature. Theoretically, the TAC may vary between 0 (implying no energy transfer between the liquid and gas upon reflection) and 1 (characterizing diffuse reemission with complete thermal equilibration of the incident gas molecules with liquid). The TAC, α_T , and the collision rate, N_g , are related to the $G_{K,cond}$ (i.e., the inverse of $R_{K,cond}$) at liquid-gas interface by [9]:

$$G_{K,cond} = fRN_g \frac{\alpha_T}{2 - \alpha_T}. \quad (4)$$

where $f = 4$ for a monatomic gas. Although Eq. (4) has been shown to give very good predictions of G_K at solid-gas interfaces [10,11], whether it is accurate or even valid in the prediction of G_K at liquid-gas interfaces remains debatable. In this work, we will test the validity and accuracy of Eq. (4) using MD simulations.

2.2. Interfacial heat transfer by evaporation/condensation

When evaporation/condensation occurs, energy is transferred by liquid-vapor phase changes at the interface. In this case, the interfacial heat flux, q , equals Jh_{fg} , where J is the evaporation/condensation rate, and h_{fg} is the latent heat. Recent MD simulations of steady state evaporation and condensation processes showed that the Schrage relationships, which were developed based on the kinetic theory of gases, accurately predict the evaporation/condensation rate, J [8,13,14]. Both the Schrage analysis and MD simulations of evaporation and condensation processes in a planar heat pipe (see Fig. 1) show that J is proportional to the temperature

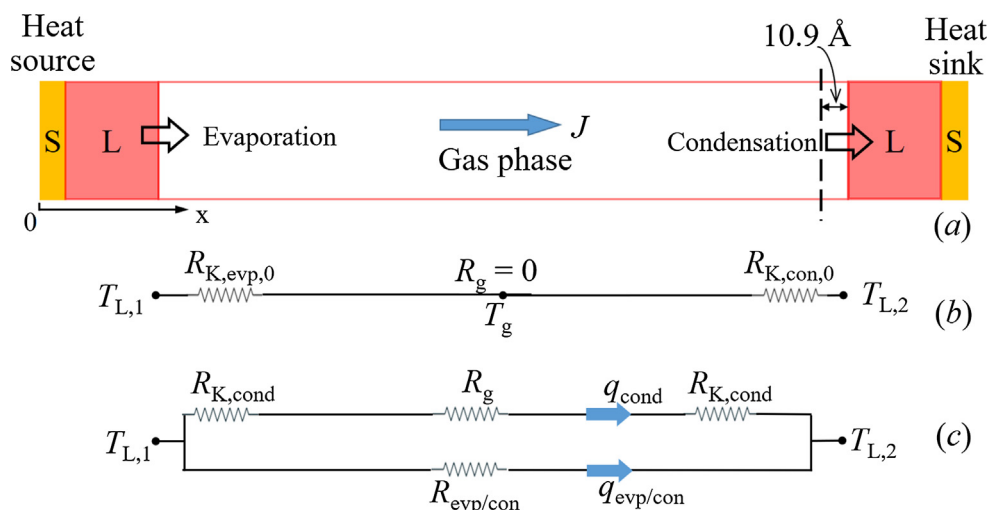


Fig. 1. (a) Schematic diagram of the model system for the study of evaporation and condensation in a planar heat pipe. S and L stand for the solid surface and the liquid phase, respectively. The vertical dashed line indicates the location of the imaginary plane (10.9 Å away from the liquid surface) for the determination of MAC. (b) The thermal resistance network between the evaporating and condensing interfaces in the heat pipe in the case of $\rho_{NCG} = 0$. (c) The thermal resistance network between the evaporating and condensing interfaces when an NCG is present in the heat pipe.

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