Switchable heat transfer in nano Janus-interface-system

Longyan Zhang [a], Jinliang Xu [a,*], Qicheng Chen [b], Sheng Wang [a]

[a] *Key Laboratory of Condition Monitoring and Control for Power Plant Equipment of Ministry of Education, North China Electric Power University, Beijing 102206, PR China*
[b] *School of Energy and Power Engineering, Northeast Electric Power University, Jilin 132012, PR China*

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ABSTRACT

Janus-interface-system is referred as liquid confined between hydrophilic and hydrophobic surfaces, nanoscale energy transfer in Janus-interface-system is not understood. Here, we investigate Poiseuille flow by non-equilibrium molecular dynamics (NEMD) using argon as the working fluid. The two solid walls hold different temperatures and wettabilities. It is found that for pure heat conduction, temperature jumps are negative on hot wall but positive on cold wall to create positive heat flow from hot wall to cold wall (called positive heat transfer). However, the convective energy transfer in Janus-interface-system always behaves positive temperature jumps on the two walls due to viscous heating. We show that, lowering hot wall wettabilities creates more significant velocity and temperature slippages on hot wall than those on cold wall to steepen liquid temperature gradients in nanochannel. We further show that heat flow sign can be switched between positive and negative, by (1) keeping super-hydrophilic hot wall but changing cold wall wettabilities, (2) keeping super-hydrophilic-hot-wall/hydrophobic-cold-wall but varying external forces applied to liquid, and (3) keeping super-hydrophilic-hot-wall/hydrophobic-cold-wall but varying hot wall temperatures. All the three cases yield non-symmetry velocity profile and more sensitive changes of temperature jumps on cold wall than those on hot wall for heat transfer switch. The transition between positive and negative heat transfer occurs at the zero temperature gradient in the channel. The findings not only enhance the understating of nanoscale energy transfer in Janus-interface-system, but also provide novel working principle for nano-devices behaving temperature sensitive nature.

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1. Introduction

Water on either hydrophilic or hydrophobic surface is a nature phenomenon. The beading-up of raindrops, on raincoats or the leaves of plants are frequently observed in our daily life [1]. If the gap between two hydrophobic surfaces becomes sufficiently small, water can be spontaneously ejected [2], whereas a water film confined in symmetric hydrophilic surfaces is stable at comparable spacings [3]. Recent attention has been paid to the behavior of water confined between one hydrophobic and one hydrophilic plate (called the Janus-interface), to learn how water reacts to the competing effects of the plates. Zhang et al. [4] studied water confined between adjoining hydrophobic and hydrophilic surfaces (a Janus-interface). They noted that whereas surface energetics encourage water to dewet the hydrophobic surface, the hydrophilic surface constrains water to be present, resulting in a flickering, fluctuating complex.

Channels using different materials involve many engineering applications. For example, a micro- or nanochannel can be formed by an etched silicon substrate bonded with a glass cover, for which wettabilities are different for the two materials. Assuming a pressure driven liquid flow in a nanochannel with asymmetric solid materials (Janus-interface-system), frictions in internal liquid film and at solid/liquid interface heat up liquid and cause nonuniform temperature distribution in the liquid. A temperature gradient in liquid is related to thermophoresis or thermodiffusion, in which suspensions tend to concentrate on either high- or low-temperature side depending on the sign of their thermodiffusivity [5,6]. This phenomenon could be used for particle and biomolecule separation through micro- or nanochannel.

Flow and/or heat transfer in nanochannel cannot be predicted by continuum medium mechanics [7]. This is because when channel size is down to micron or nano scale, the surface area to volume ratio is significantly large to induce apparent interfacial effect. Two types of boundary conditions should be treated: flow boundary condition and thermal boundary condition, which are coupled with each other to make the problem more complicated. Usually, slip

* Corresponding author.
   E-mail address: xjl@ncepu.edu.cn (J. Xu).

length L_s characterizes the degree at which the slip flow at solid-fluid interface deviates from the non-slip flow:

$$L_s = (u_l - u_w) \Big/ \frac{du}{dz}\Big|_w = \Delta u_w \Big/ \frac{du}{dz}\Big|_w \tag{1}$$

where u is the streaming velocity, Δu_w is the slip velocity at the wall, z is the coordinate perpendicular to the flow direction, the subscripts of l and w represent fluid and wall, respectively.

Numerous investigations have been performed to explore slip lengths which are dependent on solid-fluid interaction strength, shear rate and channel size [8–14]. Xu and Li [11] studied flow boundary condition over multiscale size from nano to micron or even larger. They found three types of boundary conditions (slip, non-slip and locking). Slip lengths are found to be mainly relied on solid-fluid interaction parameters, whereas channel size has almost no effect on L_s. Such finding is verified by experiments in Ulmanella and Ho [12].

Similarly, Kapitza length (L_K) characterizes the degree of temperature jump across solid-fluid interface, written as

$$L_K = (T_l - T_w) \Big/ \frac{dT}{dz}\Big|_w = \Delta T_w \Big/ \frac{dT}{dz}\Big|_w \tag{2}$$

where ΔT_w is the temperature jump at the interface. The acoustic mismatch model (AMM) is a simplified theory to explain thermal resistance at solid-fluid interface, based on the continuum acoustic wave traveling in dissimilar materials [15]. AMM treats phonons as plane waves that could be transmitted or reflected at the interface. The scattering mediated acoustic mismatch model (SMAMM) was developed from AMM, including more information about microscopic principles such as phonon scattering or radiative heat transfer [16]. However, SMAMM still employed simplified assumptions of molecular structure and their interactions, which are critical in nanoscale heat transfer. Both AMM and SMAMM have limitations to deal with thermal resistance across the interface. For example, surface wettability cannot be considered in these two models. Recent progress tends to use molecular dynamics (MD) simulation for thermal boundary treatment. MD results show that wetting liquid could enhance heat transmission across the interface, thus the Kapitza length L_K is reduced [17].

Slip velocity and/or temperature jump at the interface can be influenced by many factors such as solid-fluid interaction [18–20], solid structure [21], surface geometry and temperature [22,23], driving force [24,25], shear rate [26], temperature gradient [27]. Previous studies investigated how some of these parameters influence either slip velocity or temperature jump. Slip velocities are often studied in isothermal flows by neglecting viscous heating effect, while studies of temperature jump are conducted in pure heat conduction system without considering fluid flow [17].

In summary, flow and/or heat transfer in a Janus interface system is a nature phenomenon and involves many potential applications. The mechanism is not well understood. Previous studies involving Janus-interface-system treated flow problem only [28], while the coupling problem of flow and heat transfer was dealt with in nanochannel having identical solid materials [29–31].

Here, we investigate flow and heat transfer in a nanochannel having a liquid film confined between two walls having non-identical wall wettabilities. Non-equilibrium molecular dynamics (NEMD) method was described. The solid-liquid interaction is modelled using Lennard-Jones potential including two adjustable parameters. Changing the adjustable parameters yields different wettabilities of liquid argon on the two solid walls. Velocity and temperature fields are strongly deformed and become non-symmetry in the nanochannel. The wettability difference of the two solid walls, non-dimensional force applied to each liquid atom, and hot wall temperature are examined to influence the velocity and temperature distributions. Based on temperature gradients of liquid in the nanochannel, two regimes of heat transfer are identified: positive heat transfer (heat flow from hot wall to cold wall), and negative heat transfer (heat flow from cold wall to hot wall). The modulated heat flow direction and quantity in nanochannel can be applied for nano-system development such as biology species separator in terms of the temperature sensitive nature.

2. Non-equilibrium molecular dynamics simulation (NEMD)

2.1. MD simulation domain

Fig. 1a shows the computation problem, where *x, y* and *z* refer to axial flow direction, direction perpendicular to the paper plane and height direction, respectively. Because *g* is applied to each liquid particle, liquid argon atoms are moving along *x*. We note that *g* is a general acceleration having a unit of m/s², which may deviate from *g* = 9.80 m/s². The flow can be changed by changing *g*. The simulation box had a size of $17.15\sigma \times 11.3\sigma \times 21.2\sigma$, corresponding to $5.83 \times 3.85 \times 7.22$ nm³, where σ is the length scale of argon atom. The distance between the two walls is $H = 16\sigma = 5.41$ nm. Inside the nanochannel, there are 2340 argon atoms (at its saturated liquid density). The initial liquid density ρ and temperature *T* are 1310 kg/m³ and 100 K. The saturation liquid of argon is verified by the relationship between pressure and temperature. At the initial condition of 100 K, the pressure is 0.3277 MPa for argon, coming from the NIST software, respectively. The lattice parameter of liquid argon is determined based on its density and FCC structure, which is 1.72σ here.

We note that, liquid atoms are confined between the two solid walls. The number of liquid atoms is not changed during computation. The simulation system is a single-phase liquid system without phase change. Physical properties of liquids are mainly dependent on temperatures, weakly dependent on pressures. Liquid pressures have neglectable effect on flow and heat transfer. We also note that, different wall wettabilities yield different peak liquid densities near the wall. The peak density layer is very narrow in the channel height direction. The near-wall liquid compressibility would not change the bulk liquid densities. For a system having dense solid atoms, liquid atoms cannot penetrate solid wall. Thus, the interfacial parameters are not influenced by pressures. Pham et al. [32] studied the pressure effect on thermal boundary conditions, showing that Kapitza lengths are not changed versus pressures for a system with dense gold atoms. Feng and Liang [33] noted the neglectable effect of pressures on thermal boundary conditions for asymmetrical solid-liquid systems. Thus, it is not necessary to consider the pressure effect in this study.

The computation domain consists of a top wall and a bottom wall. Each wall includes eight layers of solid atoms. At initial computation stage, all solid atoms are arranged as a FCC lattice structure. There are 2688 platinum atoms for each solid wall corresponding to a density of 21.45×10^3 kg/m³. For each wall, solid atoms of the four layers attaching liquid film are oscillating freely. These solid atoms deviate from initial location and exchange energy with liquid atoms. Beyond the inner four layers of solid atoms, there are two layers of solid atoms acting as the thermostat atoms to keep specific wall temperature. The outmost two layers of solid atoms are stationary, which ensures the stationary of the solid wall, from macroscopic point of view. The outer four layers, including thermostat atoms and stationary atoms are called ghost atoms. The thermostat technique is implemented using following equation [34]:

$$\frac{dp_i}{dt} = -\xi p_i + f(t) + F(t) \tag{3}$$