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Micro- and nano-scale fluid flow and heat transfer with phase change in a channel

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Abstract

Micro/ Nanoscale fluid flow and heat transfer with phase change in a channel widely exist in film cooling of aircrafts and electronic devices, etc. Compared with their macroscale counterpart, Micro/ Nano-scale fluid flow and heat transfer show some new features such as velocity slip, temperature jump, density layering and non-uniform viscosity phenomena. Besides, some factors (i.e., axial conduction, viscous dissipation and rarefied effect) that are normally neglected in macroscale flow and heat transfer become dominant at Micro/ Nano-scale counterparts. In this thesis, Micro/ Nano-scale fluid flow and heat transfer are thoroughly investigated by various approaches. The two-dimensional energy equation with a first-order velocity slip model and a temperature jump model is solved analytically, and impacts of viscous dissipation, axial conduction and rarefied effect on the local Nusselt number, the asymptotic Nusselt number and the bulk temperature profile of fluid are clarified. The second law analysis method based on the local entropy generation rate is then proposed to compute and visualize the resistance of flow at low Reynolds number featuring velocity slip after implementing the linear Navier velocity slip boundary condition in OpenFOAM through three schemes. Then, classical molecular dynamics simulations are performed to reveal the features of Micro/ Nanoscale flow and heat transfer (i.e., velocity and temperature slip, non-uniform density and viscosity profiles). This study is followed by the study of the phase

change (i.e., thermal de-icing and the icephobic coatings) at the molecular level.

It is found that the asymptotic dimensionless bulk temperature of fluid converges to a constant value that is higher than the wall temperature at a given set of Brinkman number, Péclet number and Knudsen number regardless of the inlet conditions. When neglecting axial conduction and the rarefied effect, the asymptotic Nusselt number with or without viscous dissipation is 17.5 or 7.54, respectively. Effects of axial conduction on the asymptotic Nusselt number are negligible when the Péclet number is greater than 10, while its influence on the non-dimensional bulk temperature of fluid and local Nusselt number can be neglected only when $Pe > 100$. The flow resistance is caused by the wall drag force work (equal to 0 for no-slip flow) and viscous dissipation in the flow field related to the local entropy generation rate. The fully developed bulk temperature obtained from molecular dynamics simulation agrees with the continuum based solution of the analytical energy equation at channel height 24 nm , while this agreement reduces with the decrease of the height due to the nanoscale features. At height 6 nm , velocity slip exists around the hydrophobic wall, and enhanced near-wall viscosity of liquid and reduced velocity slip length are observed at larger fluid-wall interaction strength. A region around 0.2 nm wide without liquid atoms is formed at the hydrophilic wall, leading to a zero velocity in this hollow domain and a no-slip boundary condition. Most importantly, the thermal slip length is remarkably dependent on the liquid density layering in the proximity of the wall and inversely proportional to the first peak value of liquid adjacent to the interface. The energy consumption of thermal de-icing can be modelled as a bilinear function of wall temperature (T_w) and ice thickness (H). The melting time is almost bilinear with respect to H and $1/(T_w - 273.15\text{ K})$, and converges to

a constant value at $T_w \geq 313.15K$. When adopting a hydrophobic surface, which is generally considered as icephobic and prevents ice accretion, more time and almost constant energy are required to melt the ice. The ice adhesion stresses on wall substrates can be reduced significantly due to the geometrical structure, buckling phenomenon and hydrophobicity of the graphene-carbon nanotube junctions, respectively, and the reduction can be further strengthened when there is a water lubrication layer.

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Nomenclature

Greek symbols

λ	Velocity rescale factor (Chapter 1)
δf	Stochastic collision force (Chapter 1)
η	Dimensionless coordinate (Chapter 2)
γ	Friction coefficient (Chapter 1)
γ	Specific heat ratio (Chapter 2)
λ	Molecular mean free path (Chapter 2)
$\langle \delta u^2 \rangle$	Mean squared displacement (Chapter 1, 4)
μ	Dynamics viscosity (Chapter 2)
$\Phi_{cond//}$	Axial heat flux (Chapter 1)
Φ_{conv}	Total convective heat flux (Chapter 1)
ψ_1, ψ_2, ψ_3	Stochastic numbers (Chapter 1)
ρ	Density (Chapter 1, 2, 3, 4)
ρ^*	Dimensionless density (Chapter 3)
σ	Adhesion stress (Chapter 4)

σ	Length parameter in the LJ potential model (Chapter 1, 3, 4)
σ	Tangential momentum coefficient (Chapter 2)
σ_T	Thermal accommodation coefficient (Chapter 2)
θ_1, θ_2	Dimensionless temperature (Chapter 1, 2, 3)
θ_b	Dimensionless bulk temperature (Chapter 2)
ε	Energy parameter in the LJ potential model (Chapter 1, 3, 4)
$\varkappa$	Kinetic energy (Chapter 1)
ξ	Dimensionless coordinate (Chapter 2)
Pr	Prandtl number (Chapter 2)

Other symbols

$f(v_i)$	Velocity distribution function (Chapter 1)
$\boldsymbol{F}_{max}$	Maximum value of the virtual spring force (Chapter 2)
Δt	Time step (Chapter 1, 2, 3, 4)
$\dot{\gamma}$	Shear rate (Chapter 3)
$\dot{S}_{irr,D}$	Generation rate of entropy (Chapter 2)
τ_{wt}	Tangential wall stress (Chapter 2)
A	Contact area (Chapter 2)
Ag	Silver (Chapter 3)
Ar	Argon (Chapter 3)
Br	Brinkman number (Chapter 2)
c_p	Specific heat (Chapter 2)

d	Distance (Chapter 1 , 3 , 4)
E	Energy (Chapter 4)
F	Force (Chapter 1 , 2 , 3 , 4)
$f_n(\eta)$	Eigenfunctions (Chapter 2)
Gz	Graetz number
H	Hamiltonian (Chapter 1)
H	Height (Chapter 1 , 2 , 3 , 4)
K	Flow resistance coefficient (Chapter 2)
k	Spring constant (Chapter 1 , 3 , 4)
k	Thermal conductivity (Chapter 2)
K_s	Spring constant (Chapter 3)
L_{slip}	Velocity slip length (Chapter 2)
L_T	Thermal slip length
L_v	Velocity slip length (Chapter 3)
m	Mass of an atom (Chapter 1 , 3 , 4)
MSD	Mean squared displacement (Chapter 4)
N	Number of atoms (Chapter 1 , 3 , 4)
Nu	Nusselt number (Chapter 2)
p	Pressure (Chapter 1 , 2)
p_k	Momentum (Chapter 1)
Pe	Péclet number (Chapter 1 , 2 , 3)

Q	Tetrahedral order parameter (Chapter 4)
r	Distance (Chapter 1, 3, 4)
r_c	Cut-off distance (Chapter 1, 3, 4)
Re	Reynolds number (Chapter 1, 2)
S_k	Translational tetrahedral order (Chapter 4)
T	Temperature (Chapter 1, 2, 3, 4)
t	Time (Chapter 1, 2, 3, 4)
T_b	Bulk temperature (Chapter 2)
T_i	Temperature (Chapter 2)
T_w	Wall temperature (Chapter 2)
U	Potential energy (Chapter 1, 3, 4)
u	Velocity (Chapter 2)
u^*	Dimensionless velocity (Chapter 2)
u_{ave}	Average velocity (Chapter 2)
v	Velocity (Chapter 1, 2, 3, 4)
W_{drag}	Drag work (Chapter 2)
x	x coordinate (Chapter 2)
y	y coordinate (Chapter 1, 2, 3, 4)
z_n	Eigenvalues (Chapter 2)

Physics constants

k_B	Boltzmann's constant (Chapter 1, 3, 4)
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Chapter 1

Introduction

1.1 Micro- and nano-scale flow characteristics

Micro- and nano-scale flow and heat transfer problems widely exist in biological systems (i.e., kidneys, brain, blood vessels, lungs) and many man-made systems such as desalination units, heat exchangers, nuclear reactors, etc. When the channel size becomes smaller, some of the conventional classical theories of the bulk fluid, mass and energy transport become less valid. The deviation from the “conventional” theories at the microscale is caused by several rationales such as (a) the change in the fundamental process such as the deviation from the continuum assumption and the increased influence of some additional forces; (b) uncertainty regarding the applicability of some empirical factors calculated from larger scales experiments such as entrance and exit loss coefficients of pipe flow; (c) uncertainty of measurements at the microscale, such as geometrical dimensions and operating parameters ([Kandlikar et al., 2005](#); [Hetsroni et al., 2005b](#); [Liang](#)

and Mudawar, 2019). These factors also pose many scientific challenges in using numerical simulation to investigate the micro- and nano-scale flow and heat transfer. First, the validity of the well-known continuum-based Navier-Stokes equations should be revisited. Second, the no-slip boundary conditions widely applied in macroscale flow and heat transfer simulations may be invalid due to the fact that the molecular mean free path and the channel/pipe dimensions are of the same order of magnitude. Third, some factors' influences become significant, i.e, viscous dissipation that is generally neglected in macroscale heat transfer has to be considered in micro- and nano-scale flow and heat transfer.

As an important parameter, the determination of the flow resistance of micro- and nano-scale velocity slip flow is a vital issue in the process of design and fabrication of efficient microfluidic devices (i.e., micro-electro-mechanical systems (Lee et al., 2002), heat exchangers (Sheikholeslami et al., 2019) and cooling of electronic chips (Radwan et al., 2018)). For fully developed laminar pipe flow without velocity slip, it is known that the Darcy friction factor (flow resistance coefficient is proportional to the friction factor in a straight pipe/channel) is $64/Re$ (Darcy, 1857; Valougeorgis, 2007; Tao, 2009; Calzetta, 2009; Cerbus et al., 2018). This value was also reported in the well-known Moody diagram, stressed by Moody as independent on the wall relative roughness in laminar flow (Moody, 1944). Kim (Kim, 2016) reported that this value can be predicted by the classic macroscopic theory in microscale flow and concluded that scale effects do not influence the flow resistance coefficient.

However, a number of experimental measurements of the flow resistance in the laminar flow regime do not agree with each other and even show significant discrepancies (Oliveira et al., 1998). After performing a series of experiments, Qu et al. (Qu et al., 2000) observed that the friction factor

of laminar flow in microchannels with various shapes and dimensions is larger than the one obtained from the macroscale theory. On the contrary, the friction factor was found to be less than its macroscale counterpart by other researchers (Ou et al., 2004; Choi et al., 2006; Joseph et al., 2006; Ewart et al., 2007; Demsis et al., 2009). There have been no conclusive explanations of these significant discrepancies. Some works attributed these to the flow separation (Ho and Tai, 1998), the dependence of viscosity on the channel size or other physical effects which become significant in small-scale ducts (Clasen and McKinley, 2004) and so on. We believe that the following factors are also involved:

Firstly, the non-slip boundary condition on the wall becomes less valid as a significant velocity slip has been observed (Thompson and Troian, 1997; Péméja et al., 2019; Seo and Mani, 2016; Chattopadhyay et al., 2017) when the characteristic length of the channel is reduced. This is because the fluid slips when the molecular attraction between the fluid and the solid surface is reduced as the free surface energy of the solid becomes very low. Watanabe et al. (Watanabe et al., 1999) conducted experiments on water flow through square and rectangular ducts and pipes with highly water-repellent walls producing velocity slip boundary conditions and observed the maximum drag reduction ratio could reach up to 20% for square ducts and 14% for pipes. This observation offers potential explanations on the overestimation of the friction factor at extremely small scales by the macroscale theory aforementioned in the literature.

Also, the friction factor of laminar flow in micro-level ducts has been reported to be dependent on the relative roughness of the solid wall (Gloss and Herwig, 2009), contradicting the Moody diagram (Moody, 1944). Gloss et al. (Gloss and Herwig, 2009) conducted experiments to test laminar flow in microchannels with length $130\ \mu m$, height from $20\ \mu m$ to $400\ \mu m$ and rel-

ative roughness ranging from 0 to 1. Their outcomes demonstrate that the classic macroscale no-slip theory underestimates the friction factor because an increased dissipation rate near the roughness element causes more pressure loss compared with smooth wall surfaces.

Flow resistance is also dependent on the geometry variations, such as an SCC, as has been investigated in macroscale flow with applications including injection moulding, extrusion, thermoforming and polymer melt processing. A wide range of investigations including theoretical analyses ([Owens and Phillips, 2002](#)), numerical simulations ([Sunarso et al., 2007](#)) and experiments ([Boger and Walters, 2012](#)) were conducted for flow in an SCC with various contraction ratios. It should be pointed out that almost all these studies were on the effects of contraction ratio or wall slip on the flow behaviors (i.e., size and intensity of vortex, vortex shape and streamlines) of non-Newtonian fluids. No studies on the flow resistance coefficient of contraction pipe/channel flow of Newtonian fluids with a wall slip boundary condition have been performed to the best knowledge of the authors.

The flow resistance coefficient is commonly computed from pressure loss by solving the Bernoulli or Navier-Stokes (NS) equations. Celata et al. ([Celata et al., 2006](#)) observed that the viscous heating could be applied to determine the resistance coefficient of microchannel no-slip flow and validated this in their experiments. Naterer et al. ([Naterer and Camberos, 2008](#)) reported that the loss of available work could be directly related to the entropy generation by comparing the viscous dissipation term in the mechanical energy equation with the volumetric rate of entropy generation equation firstly proposed by Bejan ([Bejan and Kestin, 1983](#)). The method based on the entropy generation is called the second law analysis (SLA), referring to the second law of thermodynamics. The SLA has been widely

used in the optimal design of fluid engineering systems (Bo and Celani, 2013), analyzing the flow resistance for no-slip flow, where the drag work on the surface is zero (Herwig and Schmandt, 2014). Compared with the common NS method, the SLA gives a direct physical interpretation of the flow resistance by revealing the distribution of the energy loss over the entire flow domain, as well as the drag work along the surface.

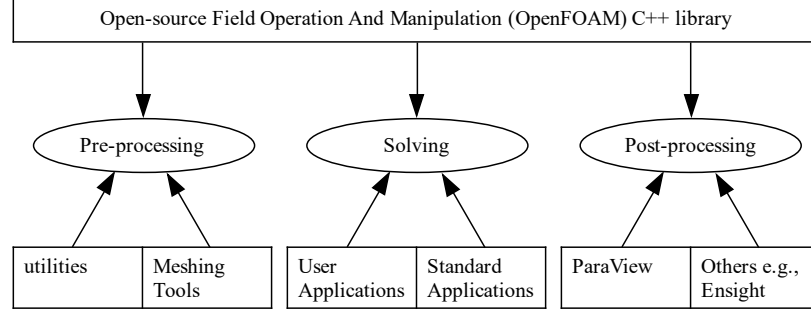


Figure 1.1: Overview of OpenFOAM structure.

In this thesis, the resistance of micro-scale flow is investigated based on the Open-source Field Operation And Manipulation (OpenFOAM). It is a framework for developing "application" executables that use packaged functionality contained within a collection of approximately 100 C++ libraries. OpenFOAM is shipped with approximately 250 pre-built applications that fall into two categories: "solvers", that are each designed to solve a specific problem in fluid (or continuum) mechanics; and "utilities", that are designed to perform tasks that involve data manipulation. The solvers in OpenFOAM cover a wide range of problems in fluid dynamics.

Users can extend the collection of solvers, utilities and libraries in OpenFOAM, using some pre-requisite knowledge of the underlying method, physics and programming techniques involved. OpenFOAM is supplied with pre- and post-processing environments. The interfaces to the pre- and post-processing are themselves OpenFOAM utilities, thereby ensuring consistent data handling across all environments. The overall structure

of OpenFOAM is shown in Fig. 1.1 (see <https://cfd.direct/openfoam/> for more details about this software).

1.2 Micro- and nano-scale heat transfer

Micro- and nano-scale heat transfer has drawn significant attention due to the rapid development of micromechanics in the last decades and its engineering applications (Ho and Tai, 1998; Gad-el Hak, 1999; Cerri et al., 2007; Zhao et al., 2016). For example, the miniaturization and the ultra-high processing speed of chips can cause a very high-heat flux, and the temperature of the hotspots resulted from such high heat flux is dramatically higher than the average temperature of the chip (Ji and Yan, 2008). These hotspots pose a thermal bottleneck for the overall reliability of chips, which increases the demand for cooling by using fluid or gas flow through channels (Wu et al., 2019). Also, nanopore membranes and nanotube attracting many researchers' attention have high water permeability and solute exclusion, and can be used to reduce the size of the desalination system and improve the energy efficiency by imposing a small temperature difference (Zhao and Wu, 2015). Experiments have shown that flow and heat transfer characters in the microchannel are quite different from their well-known macroscale counterparts (Choi, 1991; HARLEY et al., 1995) due to the following factors: (1) No-slip velocity, no-slip temperature boundary conditions and even the continuum assumption widely used in macrochannel fluid flow and heat transfer governing equations become less valid as the size of the channel is reduced. (2) In microchannel or nanochannel, the molecular mean free path is in the same order as that of channel size, which requires the consideration of molecular effects on heat transfer. (3) A series of distinct molecular layers form the density layering in the vicinity of the

fluid-wall interface and produce the non-uniform density ([Gruener et al., 2016](#)) and viscosity ([Vo et al., 2015](#)) profiles.

1.2.1 Parameter dependence of the heat transfer

The axial conduction and viscous dissipation which are generally neglected in macroscale flow and heat transfer problems are not trivial in microscale or nanoscale heat transfer. Hence, significant efforts have been devoted to studying the parameter dependence of the heat transfer. For example, Tso et al. ([Tso and Mahulikar, 1998, 1999, 2000](#)) performed dimensional analyses and experiments to show the impact of the Brinkman number on the microchannel flow. Their results stated that the Brinkman number has an essential role in determining the flow transition point and the temperature distribution in spite of its relatively small values. Tunc et al. ([Tunc and Bayazitoglu, 2001](#)) studied the effect of viscous dissipation on the heat transfer of microtubes with uniform temperature and uniform heat flux via the integral transform technique and they obtained the asymptotic Nusselt number at prescribed Knudsen number, Brinkman number and Prandtl number. The same authors ([Tunc and Bayazitoglu, 2002](#)) also applied the H2-type boundary condition to analyze viscous dissipation influences on the temperature field in a rectangular channel at constant axial and wall normal heat flux and obtained similar results as in circular microtubes. Koo et al. ([Koo and Kleinstreuer, 2004](#)) used dimensional analyses and numerical simulations to reveal the effects of viscous dissipation on the temperature profile and friction factor for three working fluids (water, methanol and isopropanol) with various conduit geometries and showed that viscous dissipation cannot be neglected in flow in micro conduits.

A series of analytical solutions for heat transfer in a one-dimensional mi-

crochannel when only axial conduction is considered has been extensively reported (Michelsen and Villadsen, 1974; Lahjomri and Oubarra, 1999; Lahjomri et al., 2002; Weigand and Lauffer, 2004; Tiselj et al., 2004; Maranzana et al., 2004; Minkowycz and Haji-Sheikh, 2006; Haji-Sheikh et al., 2009). For example, Lahjomri et al. (Lahjomri and Oubarra, 1999; Lahjomri et al., 2002) and Haji-Sheikh et al. (Haji-Sheikh et al., 2009) applied the series analysis solution method to investigate the temperature profile in parallel plate channels or circular ducts, respectively. They concluded that the effect of axial conduction influence needs to be considered when $Pe < 10$. Minkowycz et al. (Minkowycz and Haji-Sheikh, 2006) also adopted this approach to analyze heat transfer in saturated porous passages. Both experiments and numerical simulations were applied by Tiselj et al. (Tiselj et al., 2004) to obtain axial conduction effects on heat transfer characters for water flow through a triangular channel at various Reynolds numbers. The wall temperatures obtained from these two methods have a good agreement and the local Nusselt number along the flow direction has a singular point whose location is a function of the Reynolds number. The bulk temperature of water exceeds the temperature of the heated wall after this singular point. Maranzana et al. (Maranzana et al., 2004) proposed two analytical models that were utilized to analyze the influence of axial conduction on the wall using a new non-dimensional number M ($M = \frac{\Phi_{cond//}}{\Phi_{conv}}$, $\Phi_{cond//}$ is wall axial heat flux and Φ_{conv} is the total convective heat flux.). They found that the wall heat flux density becomes quite non-uniform when the Reynolds number is small and the heat transfer coefficient for small flow rates may be underestimated when using experimental data with a one-dimensional model to measure this coefficient. Gu et al. (Gu et al., 2016) analyzed axial conduction impacts on convective heat transfer via the molecular dynamics simulation method and believed that its influence should be considered in the range of $Pe < 10$. However, Hennecke(Hennecke, 1968) stated that

axial conduction might be neglected for the end of the domain in channels if $Pe > 20$.

Shah et al. (Shah and London, 2014) reviewed previous works on the joint effect of axial conduction and viscous dissipation on heat transfer in ducts. Nield et al. (Nield et al., 2003) investigated the effects of axial conduction and viscous dissipation on forced heat transfer in a porous medium with a constant temperature boundary condition and they obtained an analytical expression for the local Nusselt number as a function of non-dimensional numbers (Darcy number, Péclet number and Brinkman number). Hetsroni et al. (Hetsroni et al., 2005b) also considered viscous dissipation and axial conduction (on the fluid and the wall, jointly and separately.) effects on microtube hydrodynamics in asymptotic incompressible flow with constant physical properties via assuming $\frac{\partial T(x,y)}{\partial y} \approx 0$ (this means fluid temperature profile is 1D). In order to show the local Nusselt number distribution as a function of non-dimensional parameters (Knudsen number, Péclet number and Brinkman number), Jeong et al. (Jeong and Jeong, 2006) solved the 2D non-dimensional energy equation using a segregation variable method to make the dimensionless temperature equal to the sum of an asymptotic temperature θ_1 and another variable θ_2 . The latter variable can be expanded as an infinite series of eigenfunctions. These eigenfunctions and their coefficients in the infinite series can be computed by invoking the shooting method and the Galerkin method, respectively. Nevertheless, the exact mathematical expression of temperature was not given. Cetin et al. (Cetin et al., 2008) adopted first-order velocity slip model without a temperature jump in order to address the 2D energy equation of fluid flow in microtubes including viscous dissipation, axial conduction and rarefaction via a coordinate transformation approach (Verhoff and Fisher, 1973; Yang and Ebadian, 1991). This may not precisely mimic convective heat transfer

since fluid temperature jump is general in the vicinity of the wall. Barışık et al. ([Barışık et al., 2015](#)) defined a non-dimensional coordinate system. Then, the energy equation was solved analytically in this new dimensionless coordinate system. It was found that, when the viscous dissipation is neglected, axial conduction effects need to be considered as the Péclet number is less than 100. Haddout et al. ([Haddout and Lahjomri, 2015](#)) decomposed the energy equation into a system of the first-order partial differential equations and then solved the latter in order to show the effects of axial conduction, viscous dissipation and pressure work on heat transfer of a gaseous slip flow. They indicated that the effects of axial conduction on heat transfer should be considered in the range of $Pe < 10$ as reported by ([Lahjomri and Oubarra, 1999](#); [Lahjomri et al., 2002](#); [Haji-Sheikh et al., 2009](#); [Gu et al., 2016](#)). Clearly, a consensus for the axial conduction impacts on heat transfer has not been reached.

1.2.2 De-icing

As an interesting research topic of heat transfer, de-icing has great importance because an excessive accumulation of ice can cause devastating effects to roads, vehicles and structures. According to statistics, around 30% of the traffic accidents in the winter have resulted from the accumulation of ice on the railroad and bridge surfaces, and the corresponding economic loss can reach up to hundreds of millions of dollars per day ([Kim et al., 2015](#); [Mauro and Grossman, 2017](#)). Also, due to the low atmospheric temperature ranging from $-40\text{ }^{\circ}\text{C}$ to $0\text{ }^{\circ}\text{C}$, the icing phenomenon appears frequently at the leading edges of wings, rotor blades and propellers when the water droplets in clouds impinge on the aircraft ([Yongqiang et al., 2018](#); [Janjua et al., 2018](#)). The ice accretion can dramatically reduce the engine and

propellers' efficiency, and affect aerodynamic characteristics of the aircraft (i.e., decreasing the lift and increasing the drag force) (Bragg et al., 2005). These effects then pose a serious threat to flight safety and may lead to flight catastrophes. Therefore, over the last several decades, a variety of active and passive de-icing and anti-icing methods have been explored.

One popular active approach was to exploit chemical reactions by e.g. adding salt to the ice to reduce the freezing temperature of water, and so far over 30 million tons of salt has been employed, leading to environmental pollution and damages to vehicles (Sun et al., 2018). Most importantly, the ice could not be melted by the salt when the temperature was below -3.9°C (Chen et al., 2011). As an alternative, the environmentally-friendly thermal ice removal technique has been also actively discussed. Mauro et al. (Mauro and Grossman, 2017) tested to use the geothermal energy to melt the ice by inserting a high thermal conductivity material (e.g., aluminum) in the ground as a pathway for the spontaneous transfer of the geothermal energy to the street surface. Li et al. (Li et al., 2013a) designed a self-de-icing road system via combining the carbon nano-fiber polymer thermal source and some high thermal conductive composites, and performed experiments on the melting time and energy consumption. Liu et al. (Liu et al., 2017) proposed the design and operation parameters for the electric heating pipes employed to melt ice on the pavement. Liu et al. (Liu and Hu, 2018) conducted a theoretical analysis and experimental investigation on the heat transfer process of ice accreting on the airfoil surface. They concluded that the convective heat transfer process could be enhanced by the ice accreting near the leading edge of aircraft wings, and the ice accumulation could also be further promoted by the enhanced convective heat transfer. Karim et al. (Karim et al., 2018) produced the graphene-coated glass roving that has low energy cost and high thermal conductivity, and

could be used in various thermal de-icing applications.

On the other hand, the active de-icing techniques including thermal, mechanical, and chemical approaches are also known to have high costs and environmental drawbacks (Menini and Farzaneh, 2011). An alternative is the passive de-icing or anti-icing method that has been of great interest because it does not need the external energy input or control (Menini and Farzaneh, 2011). Such methods mainly reduce the adhesion stress and even prevents the ice formation by fabricating nonwetting surfaces (Guo et al., 2012; Kim et al., 2012), modifying the topography of surfaces (i.e., laser surface texturing, photolithography) (Ghalimi and Farzaneh, 2015), and/or coatings (Bharathidasan et al., 2014), etc. (see reference (Schutzius et al., 2015) for more details).

Three types of coating are typically applied to prevent ice accumulation on wall surfaces: coatings with very low surface energy (i.e., silicone-based or Polytetrafluoroethylene-based polymers (Croutch and Hartley, 1992), with the former one outperforming the latter one), composite/heterogeneous coatings (i.e., Croutch et al. (Croutch and Hartley, 1992) stated that the ice adhesion stress can be reduced by mixing fluorocarbon and polysiloxane type of materials), and porous/superhydrophobic coatings (Menini and Farzaneh, 2011). Inspired by animals and plants who remove dirt from their superhydrophobic surface via the motion of water drop, many superhydrophobic materials (i.e, created by primary porous structures, a low surface energy thin film (Saleema and Farzaneh, 2008) or hydrophobic molecules such as micro- and nano-scale fibers (Zhang et al., 2004)) have been developed for ice prevention. For example, a superhydrophobic surface can be produced by introducing micro- and nano-scale structures to the substrate surface with hydrophobic coatings created by coating the base surface with compounds containing low surface energy components

(Davis et al., 2014). A significant reduction of ice adhesion stress has been observed for the obtained superhydrophobic structure. However, Varanasi et al. (Varanasi et al., 2010) argued that an upward trend of ice adhesion strength exists for the superhydrophobic surfaces due to the existence of frost, and similar observations were also reported by other researchers (Chen et al., 2012; Zou et al., 2011) owing to various mechanisms. For example, Chen et al. (Chen et al., 2012) attributed the ineffectiveness and even negative effects of superhydrophobic surfaces on reducing the ice adhesion stress to the mechanical interlocking between the ice and the surface texture.

Despite the recent progress, there are several interesting and vital issues for the active and passive anti-icing methods that have still not been tackled.

(1) Although the thermal de-icing was extensively studied in previous macroscale experiments, there are no approximate equations for the melting time and energy consumption, and snapshots taken by camera cannot accurately show the interface between the ice and water during the melting process.

(2) The effects of the wall wettability on the melting have rarely been investigated thoroughly.

(3) The manufacture of composite/heterogeneous coatings is an exceptionally challenging task.

To address these points, multi-layers of graphene sheet and the G-CNTs are proposed, and numerical simulations are performed to fully investigate the thermal de-icing and these novel icephobic coatings.

1.3 Molecular dynamics simulation

It should be pointed out that although tremendous effort introduced in Section 1.2 has been devoted to investigating the micro- and nano-scale heat transfer using the continuum-based energy equations with velocity and thermal slip wall boundary conditions, the applied slip model contains constant momentum and thermal accommodation coefficients, which, unfortunately, strongly depend on materials of fluids and the wall, local pressure, velocity and the mean direction of the local flow (Karniadakis et al., 2006). Consequently, these factors may lead to the breakdown of the continuum-based model in depicting the heat transfer at micro- and nano-scale.

Moreover, the de-icing issue has also been widely investigated in numerical simulations and experiments from the macro level, as mentioned in Section 1.2.2. However, the underlying physical mechanisms (i.e., the transition to the disordered state) (Mochizuki et al., 2013) of the thermal de-icing and the ice/water equilibrium were very difficult to observe and clarify by those efforts (Kim and Yethiraj, 2008).

The molecular dynamics (MD) simulation has become an effective alternation to study the micro- and nano-scale fluid, heat transfer characteristics and de-icing as it does not introduce any postulation except the potential functions describing the interforce of particles (Fan et al., 2015; Sahebi and Azimian, 2019; Mochizuki et al., 2013; Donadio et al., 2005; Ji and Yan, 2008). For molecular methods, the presence/absence of velocity or thermal slip in the vicinity of a solid wall comes out as part of the answer. The thermal properties of materials in the system and system-level transport properties can be computed from the resulting kinematic trajectories and inter-molecular forces. Also, there is no need to consider whether the

fluid is Newtonian/non-Newtonian or Fourier/non-Fourier. With these advantages, molecular dynamics simulation has become an effective tool for investigating molecular transport and heat transfer ([Rapaport, 2004](#); [Allen and Tildesley, 2017](#)).

The MD simulation begins with a set of N molecules in a region of space, and each of the particles is assigned a random velocity corresponding to a Boltzmann distribution at the temperature of interest. The interaction between the particles is prescribed typically in the form of a suitable potential energy and the time evolution of the particles' positions is determined by integrating Newton's equations of motion, one for each molecule. Hydrodynamic and thermodynamic parameters can be obtained by artificially dividing the flow domain into bins and then count velocity information, etc. of every particle in that bin.

1.3.1 Initialization of particles' velocities and positions

Before starting a molecular dynamics simulation, particles' velocities need to be initialized and their velocities can be assigned to random numbers according to the Maxwell velocity distribution which is a Gaussian profile with standard deviation $\sigma = \left(\frac{KT}{m}\right)^{\frac{1}{2}}$ and the mean value $\langle v_i = 0 \rangle$ ([Haile et al., 1993](#))

$$f(v_i) dv_i = \frac{N(v_i) dv_i}{N} = \sqrt{\frac{m}{2\pi k_B T}} \exp\left(-\frac{mv_i^2}{2k_B T}\right) dv_i, \quad i = 1, 2, 3 \quad (1.1)$$

where $f(v_i)$ is the velocity distribution function, N is the total number of

atoms and k_B is the Boltzmann's constant.

Particles' positions can be initialized to random numbers or concrete crystal structures such as hexagonal close-packed (hcp), face-cantered cubic (fcc), body-cantered cubic, (bcc) and simple cubic (sc), etc. as shown in Fig. 1.2.

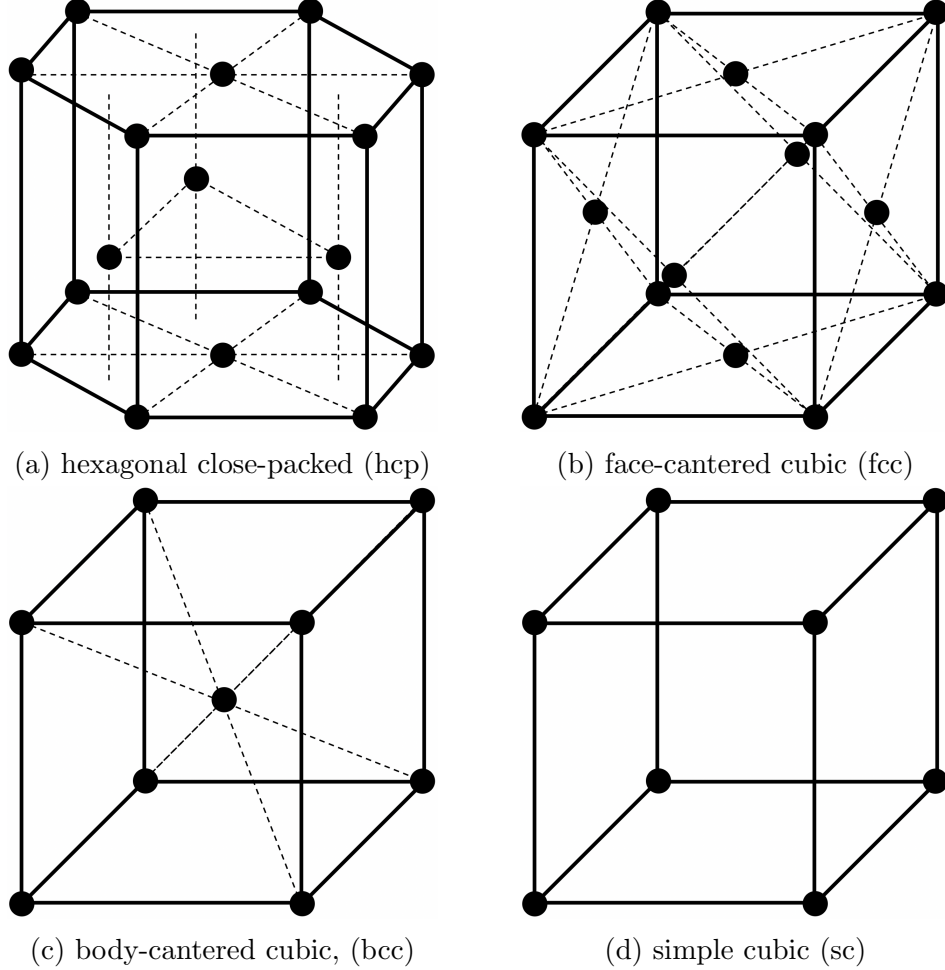


Figure 1.2: Crystal structures.

1.3.2 Streamwise boundary conditions

In the molecular dynamics method simulation of flow and heat transfer, boundary conditions can be roughly divided into two categories: periodic boundary conditions and non-periodic boundary conditions.

Stream-wise periodical boundary conditions which have been widely used

in the flow direction as it is conservative, robust, efficient and very straightforward to implement in a molecular simulation program (Müller-Plathe, 1997; Li et al., 1998; Sokhan et al., 2001; Rapaport, 2004; Allen and Tildesley, 2017), are manifested in two separate two ways. First of all, they are manifested in the trajectories of atoms or molecules. Secondly, they are manifested in the ‘minimum image convention’ in determining the amplitude of the distance of arbitrary two particles, and the amplitude of the distance can be applied to calculate forces, kinematic energy or internal energy, etc.

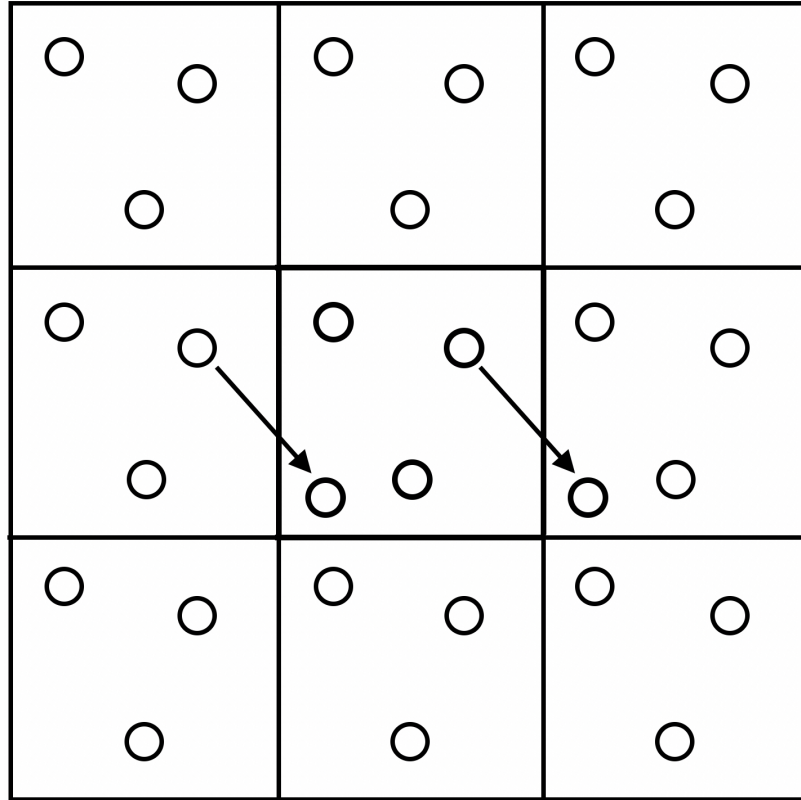


Figure 1.3: Periodic boundary conditions. When a particle leaves the modelling domain, a corresponding image particle of this particle enters the simulation zone.

It should be pointed out that periodic boundary conditions are often applied in the simple geometric model. For some relatively sophisticated geometric model, for example, the shapes of inlet and outlet of the inves-

tigated micro-channel or nano-channel are different, periodical boundary conditions maybe not be applied in these cases. Matthew K. Borg etc. proposed a stream-wise non-periodical boundary condition model which was applied to study flow in arbitrary geometries (Borg et al., 2010).

Nicholls et al. (Nicholls et al., 2012) and Docherty et al. (Docherty et al., 2014). employ separately this non-periodical boundary condition to simulate water transport through carbon nanotubes. In this boundary condition, the upstream pressure of the micro duct is controlled by a PID feedback loop algorithm. It applies an external body force that includes three separate components (a proportional term, a derivative term and an integral term) to all particles in a user-defined control domain. Meanwhile, the adaptive control is taken to compensate for any particles leaving the system. The pressure flux technique is performed to control the pressure of the duct downstream (De Fabritiis et al., 2006). All of these techniques can ensure that the flow in the micro duct develops naturally without any over-constraint.

1.3.3 Wall boundary conditions

In molecular dynamics simulations, the most frequently used wall boundary conditions are:

(1) Structure-less reflection model

In this condition, the effect that each solid wall atom acts on the liquid/gas atom in the nano-scale channel is neglected totally.

(a) Specular and diffuse reflection wall model

To describe interactions of gas molecules with the surface, Maxwell et al.

(Maxwell, 1878) described specular and diffuse reflection models in 1897, which were appropriate in kinetic theory-based approaches proposed by Bird et al. (Bird and Brady, 1994). In this wall approach, a fraction α (this fraction is named the accommodation coefficient) of the incident particles are reflected diffusely and the rest of particles experience specular reflection. Compared with a stochastic thermal wall scheme, a particle recoil from the wall surface at an arbitrary random velocity rather than a velocity that is closely related to the wall temperature.

(b) Stochastic thermal wall model

Sun and Ebner (Sun and Ebner, 1992) used a stochastic thermal wall model considering the interactions between the fluid/gas particles and the wall. When a liquid/gas atom strikes on the solid wall that confines all liquid/gas atoms, it will rebound at a stochastic velocity that is unrelated to its initial velocity (Tehver et al., 1998). The random velocity following the Gaussian distribution is determined by the wall temperature. Three velocity components of a liquid/gas atom rebounding from a solid wall is (assuming that two solid walls are perpendicular to z axis and parallel to xy plane) (Alexander and Garcia, 1997):

$$v_x = \sqrt{\frac{k_B T_w}{m}} \psi_1 \quad (1.2a)$$

$$v_y = \sqrt{\frac{k_B T_w}{m}} \psi_2 \quad (1.2b)$$

$$v_z = \pm \sqrt{\frac{k_B T_w}{m}} \psi_3 \quad (1.2c)$$

If a particle striking on the top wall plane, then the negative sign should be chosen. This scheme can prevent liquid/gas particles from passing through solid walls to maintain the number of liquid/gas particles as a constant value. ψ_1 and ψ_2 are stochastic numbers following the Gaussian distribution

with zero mean value and unit variance. ψ_3 is also a random number obeying a uniform distribution in (0,1). This wall model enables the energy transfer between the wall and fluid/gas particles. It, however, presented obvious difficulties in implementing the moving boundaries. More details about the algorithm of particles rebounding from the solid wall are reported in reference (Tenenbaum et al., 1982; Song and Chen, 2008).

(2) Structured wall model

In this model, the wall consists of a series of realistic particles rather than some imaginary boundaries utilized in simple specular and diffuse reflection and stochastic thermal wall model. All solid wall atoms are frequently arranged at a simple cubic lattice or face-centered lattice (FCC). The interaction between solid wall atoms and liquid/gas atoms in the nano-channel can still be modelled by the Lennard-Jones potential which will be introduced detailly in the following section. According to whether solid wall atoms are stationary or oscillatory, this model includes stationary and Harmonic spring wall models.

(a) Stationary wall atoms

All solid wall atoms are constrained to their corresponding initial positions in the whole process of molecular dynamics simulation. Liquid/gas particles collide (interact) with these wall particles, and inter-molecular forces are determined by the type of intermolecular potential energy function (Mountain and MacDonald, 1983; Thompson and Robbins, 1990; Thompson and Troian, 1997).

Two ways can be used to fix wall particles in their initial lattice positions. Wall particles' velocities and external forces from liquid/gas particles can be artificially set as zero. Alternatively, instead of fixing all wall particles

in their initial positions in the whole process of modelling, it is possible to artificially assume extreme heavy mass (e.g. $m_{wall} = 10^9 m_{fluid}$) to wall particles so that these wall particles with zero velocities are nearly stationary even though they undergo forces from other atoms or molecules (Koplik et al., 1989).

(b) Harmonic spring wall model

Cieplak et al. proposed a more realistic solid wall boundary condition to describe interactions between solid wall atoms and liquid/gas particles at the wall–fluid interface (Cieplak et al., 2001). That is, all wall particles are constrained to their initial lattice positions via using harmonic springs (this harmonic spring model is also in chemical bond of protein molecules in molecular dynamics modelling of hydrodynamical and thermodynamic problems (Hansen and McDonald, 1986; Bitsanis et al., 1987; Travis et al., 1997; Bernardi et al., 2010; Marable et al., 2017)), which allows the wall particles to oscillate freely.

The spring force that constrains wall atoms to their original positions is

$$F = kr, \tag{1.3}$$

where k is the spring constant and r is the distance that a solid wall particle deviates its initial position.

Cieplak et al. used a spring with high stiffness constant to constrain the displacements of the vibrating wall particles (Cieplak et al., 2001). However, the over-constraints of the wall particles can cause the viscous heating of liquid/gas particles, and the heat has to be dissipated by applying the thermostat algorithm to maintain the temperature of liquid/gas particles in equilibrium. The heat interactions between the fluid/gas particles and

wall surfaces were not modelled adequately (Kim et al., 2008b).

Consideration must be taken when adopting the spring constant k to maintain that: (1) wall boundary structures are well-defined with a minimum number of particles; (2) the nearest neighbouring distance between solid wall atoms is small enough to prevent fluid particles leaking through the wall (Powles et al., 1992); (3) wall particles are not over-constrained during the process of molecular dynamics simulation.

Hansen et al. (Hansen and McDonald, 1986) and Thompson et al. (Thompson and Robbins, 1990) believed that the parameter could be chosen according to the Lindemann criterion widely used in molecular dynamics simulations (Khare et al., 1996, 1997, 2001).

$$\frac{\langle \delta u^2 \rangle}{d^2} \leq 0.023, \quad (1.4)$$

where $\langle \delta u^2 \rangle$ is the mean squared displacement about the lattice sites and d is the nearest-neighbour distance. However, it is complex to determine the spring constant through the Lindemann criterion due to that some parameters in this rule have to be obtained from neutron scattering experiments.

Khare et al. (Khare et al., 2006) also reported a relatively straightforward method to estimate the spring constant.

$$k = \frac{500\varepsilon}{\sigma^2}, \quad (1.5)$$

where ε and σ are the energy character parameter and length character parameter in the LJ potential energy model, respectively. The criteria was extensively applied in previous work (Ge et al., 2015; Gu et al., 2016; Marable et al., 2017; Papanikolaou, 2017). Hence, in this thesis, we com-

pute the spring constant parameter based on Eq. (1.5).

1.3.4 Potential energy functions

As illustrated before, the only input that should be provided by users in molecular dynamics simulation is the potential energy function which quantitatively describes interactions among particles. The form of potential energy function has to be obtained from a subatomic theory of physics and chemistry according to the concrete type of particle, and parameters in potential energy function are fitted either from experimental results or quantum calculation data.

The potential energy is conventionally classified into intermolecular and intramolecular components. The intramolecular forces that should be computed when the molecules have non-negligible internal degrees of freedom consist of

1. chemical bond-stretching
2. bond-bending
3. bond torsion around a dihedral angle.

The intermolecular interactions include

1. electron cloud repulsion
2. attractive van der Waal's dispersion
3. Coulombic interactions between distinct molecules or atoms of the same molecule separated by a substantial distance (such as atoms in different parts of a polymer chain).

For simple fluids, we are interested only in the intermolecular potential generally characterized as pair-wise potentials or many-body potentials. One of the commonly used pair-wise potentials is the Lennard-Jones potential (Jones, 1924), and it is defined as

$$U = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right], \quad (1.6)$$

where r is the magnitude of the distance between two arbitrary particles, ϵ is the well-depth of the Lennard-Jones potential and σ is the collision diameter.

Conventionally, Lennard-Jones potential parameters (well-depth ϵ and collision diameter σ) can be determined from the Lorentz-Berthelot rules (Lorentz, 1881; Berthelot, 1898)

$$\epsilon_{ij} = \sqrt{\epsilon_{ii}\epsilon_{jj}}, \quad (1.7a)$$

$$\sigma_{ij} = \frac{\sigma_{ii} + \sigma_{jj}}{2}. \quad (1.7b)$$

To maintain the computation to a reasonable level, the Lennard-Jones potential is generally truncated at a relatively short range (usually at a typical cut-off distance of $r_c = 2.5$ (in MD units (Rapaport, 2004)) through three methods including simple truncation, truncation and shift, Minimum image convention (Frenkel and Smit, 2001).

Simple truncation is the simplest method that ignores all interaction when the distance of arbitrary two particles is larger than the cut-off distance r_c . The Lennard-Jones potential is shown as follows after being

truncated with this method.

$$U = \begin{cases} 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] & r \leq r_c, \\ 0 & r \geq r_c. \end{cases} \quad (1.8)$$

It should be pointed that this truncation method may cause appreciable error in estimating the potential energy of the system of the original Lennard-Jones potential.

Truncation and shift is also a common procedure to truncate the potential, and the corresponding Lennard-Jones potential is

$$U = \begin{cases} 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] - 4\varepsilon \left[\left(\frac{\sigma}{r_c} \right)^{12} - \left(\frac{\sigma}{r_c} \right)^6 \right] & r \leq r_c, \\ 0 & r \geq r_c. \end{cases} \quad (1.9)$$

In this truncation method, the Lennard-Jones potential is continuous, and there is no impulsive correction to the pressure. Meanwhile, intermolecular forces are always finite. However, one should be much careful when using the truncation and shift intermolecular potential to model anisotropic system.

1.3.5 Integration algorithms of the equations of motion

The time-dependent particles' positions are updated by integrating Newton's equations of motion, one for each molecule. Several integration methods have been developed to solve Newton's equations such as the Verlet

algorithm, and we will review them in this section.

(a) Verlet algorithm (Frenkel and Smit, 2001)

According to the Taylor expansion, the coordinate r of a particle can be written as

$$r(t + \Delta t) = r(t) + \frac{dr(t)}{dt}\Delta t + \frac{d^2r(t)}{dt^2}\frac{\Delta t^2}{2} + O(\Delta t^3), \quad (1.10)$$

where t is the current time and Δt is the time step. Similarly,

$$r(t - \Delta t) = r(t) - \frac{dr(t)}{dt}\Delta t + \frac{d^2r(t)}{dt^2}\frac{\Delta t^2}{2} + O(\Delta t^3). \quad (1.11)$$

Then, we can obtain

$$r(t + \Delta t) = 2r(t) - r(t - \Delta t) + \frac{d^2r(t)}{dt^2}\Delta t^2 + O(\Delta t^4). \quad (1.12)$$

The truncation error of particles' new positions is of order Δt^4 . Also, it can be found that new positions of particles are not calculated from particles' velocities in the Verlet algorithm. The velocity information can be obtained from

$$r(t + \Delta t) - r(t - \Delta t) = 2\frac{dr(t)}{dt}\Delta t + O(\Delta t^3),$$

or (1.13)

$$\frac{dr(t)}{dt} = \frac{r(t + \Delta t) - r(t - \Delta t)}{2\Delta t} + O(\Delta t^2).$$

By the way, the accuracy of particles' velocities derived from the above equation is only to order Δt^2 .

(b) Leap Frog algorithm (Rapaport, 2004)

The leap frog scheme is completely equivalent to the Verlet algorithm and

it is also can be derived from the Taylor expansion

$$r(t + \Delta t) = r(t) + \frac{dr(t)}{dt}\Delta t + \frac{d^2r(t)}{dt^2}\frac{\Delta t^2}{2} + O(\Delta t^3). \quad (1.14)$$

Rewrite the above equation as

$$\begin{aligned} r(t + \Delta t) &= r(t) + \left(\frac{dr(t)}{dt} + \frac{d^2r(t)}{dt^2}\frac{\Delta t}{2} \right) \Delta t + O(\Delta t^3) \\ &= r(t) + \frac{dr(t + \frac{\Delta t}{2})}{dt}\Delta t + O(\Delta t^3). \end{aligned} \quad (1.15)$$

Similarly, velocities can also be expanded as Taylor series

$$\begin{aligned} \frac{dr(t + \frac{\Delta t}{2})}{dt} &= \frac{dr(t)}{dt} + \frac{d^2r(t)}{dt^2}\frac{\Delta t}{2} + O(\Delta t^2), \\ \frac{dr(t - \frac{\Delta t}{2})}{dt} &= \frac{dr(t)}{dt} - \frac{d^2r(t)}{dt^2}\frac{\Delta t}{2} + O(\Delta t^2). \end{aligned} \quad (1.16)$$

Then, we can obtain

$$\frac{dr(t + \frac{\Delta t}{2})}{dt} = \frac{dr(t - \frac{\Delta t}{2})}{dt} + \frac{d^2r(t)}{dt^2}\Delta t + O(\Delta t^3). \quad (1.17)$$

Therefore, particles' new coordinates can be calculated from their corresponding old positions according to Eq. (1.15), and velocities are updated based on Eq. (1.17). One should note that, in the leap frog algorithm, particles' velocities are not obtained at the same time as their coordinates. Therefore, the total energy for all particles cannot be computed from the algorithm due to that potential energy and kinetic energy are not defined at the same time.

(c) Velocity-Verlet algorithm (Frenkel and Smit, 2001)

In this algorithm, particles' positions can be updated from the following

expression

$$r(t + \Delta t) = r(t) + \frac{dr(t)}{dt}\Delta t + \frac{d^2r(t)}{dt^2}\frac{\Delta t^2}{2} + O(\Delta t^3), \quad (1.18)$$

and their velocities are updated as

$$\frac{dr(t + \Delta t)}{dt} = \frac{dr(t)}{dt} + \left[\frac{d^2r(t + \Delta t)}{dt^2} + \frac{d^2r(t)}{dt^2} \right] \frac{\Delta t}{2}. \quad (1.19)$$

This algorithm is equivalent to the original verlet algorithm.

1.3.6 Statistical sampling of thermodynamic quantities

In this section, We will report thermodynamic quantities such as temperature and pressure, etc. The total internal energy, potential energy and kinetic energy of a system can be calculated from ([Allen and Tildesley, 2017](#))

$$E = \langle H \rangle = \langle U \rangle + \langle \varkappa \rangle, \quad (1.20)$$

where H is Hamiltonian, U is potential energy and $\varkappa$ is kinetic energy. According to the virial theorem, the temperature can be computed from the following equation

$$\left\langle p_k \frac{\partial H}{\partial p_k} \right\rangle = k_B T, \quad (1.21)$$

where p_k is momentum. In the atomic case, we can obtain the energy equipartition principle:

$$2\langle \varkappa \rangle = \left\langle \sum_{i=1}^N \frac{|p_i|^2}{m_i} \right\rangle = 3Nk_B T. \quad (1.22)$$

Based on the above equation, an instantaneous ‘kinetic temperature’ is defined as

$$T = \frac{2\langle \varkappa \rangle}{3Nk_B} = \frac{1}{3Nk_B} \sum_{i=1}^N \frac{|p_i|^2}{m_i}. \quad (1.23)$$

The instantaneous pressure is defined as

$$p = \rho k_B T \left[1 - \frac{1}{3Nk_B T} \left\langle \sum_{i < j} \sum r_{ij} \frac{du(r_{ij})}{dr_{ij}} \right\rangle \right], \quad (1.24)$$

where $u(r)$ is a pairwise potential. The first term of the right side of the equation is the ideal gas contribution, and the second term is the contribution of intermolecular forces. More details about the derivation process of pressure can be seen in reference ([Haile et al., 1993](#)).

1.3.7 Thermostat methods

In molecular dynamics modelling of micro-level flow and heat transfer problem, the thermostat is a vital concept as we need to maintain temperature for some atoms at a prescribed value. In this section, we will review the commonly used thermostat algorithm including velocity rescaling, Berendsen thermostat, Andersen thermostat, Nose-Hoover thermostat and Langevin thermostat.

(1) Velocity rescaling thermostat([Plimpton, 1995](#))

As illustrated in the previous section, the temperature is computed from the velocity of each particle. Thus, the straightforward way to control the temperature at a given value is to directly rescale every particle’s velocity, which is also the core idea of the thermostat algorithm.

To explain the flowchart of this algorithm, let us assume the temperature is T_j and particle’s velocity is v_j at the j time step. Based on the energy

equipartition principle of Eq. (1.23):

$$T_j = \frac{1}{3Nk_B} \sum_{i=1}^N \frac{|p_i|^2}{m_i} \propto v_j^2. \quad (1.25)$$

If the given temperature at the $j+k$ time step is T_{j+k} , and the corresponding velocity is v_{j+k} . Similarly,

$$T_{j+k} = \frac{1}{3Nk_B} \sum_{i=1}^N \frac{|p_i|^2}{m_i} \propto v_{j+k}^2. \quad (1.26)$$

Assuming a parameter λ

$$\lambda^2 = \frac{T_{j+k}}{T_j} = \frac{v_{j+k}^2}{v_j^2}. \quad (1.27)$$

Therefore, one can rescale every particle's velocity v_j by a factor λ to maintain that velocity of per particle v_{j+k} is equal to λv_j at the $j+k$ time step so that the temperature will be equal to the prescribed temperature. This algorithm, however, does not reveal correctly the energy fluctuation in the molecular system.

(2) Berendsen thermostat

Berendsen proposed an algorithm to control the temperature of a model system to a desired value (Berendsen et al., 1984). An external bath with constant temperature is chosen to couple with the simulation system. Meanwhile, particles' velocities are modified through a time scale τ in each time step, which is similar to the velocity rescaling scheme.

Assuming that a particle's velocity is v_j at j time step and is v_{j+1} at $j+1$ time step. In this thermostat scheme, we have

$$\lambda^2 = 1 + \frac{\Delta t}{\tau} \left(\frac{T_{j+1}}{T_j} - 1 \right), \quad (1.28)$$

and

$$v_{j+1} = \lambda v_j, \quad (1.29)$$

where λ is velocity rescale factor, Δt is time step and τ is time scale.

Although this efficient thermostat scheme is widely used in molecular dynamics modelling (Longhurst and Quirke, 2007; Liu et al., 2012), it should be pointed that it does not yield a canonical probability profile in the momentum space (Karniadakis et al., 2006).

(3) Andersen thermostat

Andersen et al. (Andersen, 1980) reported a thermostat scheme that maintains the temperature of the molecular system to the desired value through applying stochastic forces. This scheme can be classified into two categories: single particle and massive collision approach. In the single particle method, one can choose a random particle and reassign all velocity components of this particle based on the Maxwell-Boltzmann distribution at the prescribed temperature. In the massive collision approach, however, the random re-assignment of every velocity component is employed for all particles in the molecular system.

In the Andersen thermostat scheme, the profile of kinetic energy, potential energy and microstate probability of a molecular system mimic the realistic form of the canonical ensemble. That is, it can yield rigorously the correct canonical ensemble probabilities.

Care must be taken that particles' diffusion constants may be not correctly calculated from this thermostat approach due to a fact that stochastic collisions leave particles' velocities to decorrelate much faster than the real situation, and the true kinetics of particles are not constant.

(4) Nose-Hoover thermostat

The Nose-Hoover thermostat is first proposed by Nose (Nosé, 1984), and then modified by Hoover (Hoover, 1985) and Nose (NOSÉ, 2002). This scheme yields canonical temperature fluctuations by affecting intermolecular forces from the extended ensemble system. It is the most popular thermostat that sustains the canonical ensemble distribution both in configuration and momentum space (Kim et al., 2008b). This approach, however, may exhibit pathological behaviour for the specific molecular system, and some schemes are being developed to refine this thermostat method.

(5) Langevin thermostat

Another thermostat method is the Langevin thermostat reported by Schneider T etc. (Schneider and Stoll, 1978a) and this method is also widely utilized in molecular dynamics simulation (Heine et al., 2005; Marable et al., 2017). The key idea of the scheme is to consider viscous effects in the governing equation of motion. The force of a particle includes contributions from a gradient of the potential energy surface and a frictional force. Thus, the equations of motion of a particle i become

$$m_i \frac{d^2 r_i(t)}{dt^2} = -\frac{\partial U(r)}{\partial r_i} - \gamma_i m_i \frac{dr_i(t)}{dt} + \delta f, \quad (1.30)$$

where γ_i is a friction coefficient. δf is a stochastic collision force that obeys the Gaussian distribution (the standard deviation is $\sigma^2 = 2\gamma_i m_i k_B T$) and its probability is

$$\rho(\delta f) = \sqrt{\frac{1}{2\pi\sigma}} \exp\left(-\frac{|\delta f|^2}{2\sigma^2}\right). \quad (1.31)$$

This thermostat scheme has obvious merits. Initially, one can choose a relatively large time step than in common molecular dynamics simulation

because the friction damping term increases the robustness of the governing equation above. In addition, fewer iterative calculations are needed due to that many particles are eliminated and included simultaneously in the stochastic term. More details about the thermostat algorithm in molecular dynamics simulations can be seen in reference ([Hünenberger, 2005](#)).

Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) developed by the Sandia National Laboratories is a classical open-source molecular dynamics simulation code distributed freely under the terms of the GNU Public License (GPL). This code provides numerous force fields (i.e., pairwise potentials, many-body potentials, coarse-grained potentials and mesoscopic potentials), ensembles (i.e., NVE, NVT, NPT and NPH), and integrators (i.e., velocity-Verlet integrator, Brownian dynamics and rigid body integration). It can run on a single processor or in parallel by adopting the distributed-memory message-passing parallelism (MPI) and spatial-decomposition method of the simulation domain. These features of the code enable the simulation of soft (i.e., polymers, biomolecules) and solid-state (i.e., semiconductors, metals) materials and coarse-grained (e.g. bead-spring polymers) or mesoscopic systems at the atomic and even mesoscale. Meanwhile, the code is designed to be easy to develop or extend with new functionality and features. Therefore, all molecular simulations in this thesis are performed based on LAMMPS.

1.4 Objectives and thesis outline

Compared with the molecular dynamics simulation, some interesting physical quantities can be obtained by performing the continuum-based analytical solution and numerical simulation over a shorter time. For example,

to predict the bulk temperature profile of the Micro/ Nanoscale channel flow, the temperature profile can be computed based on our analytical solution of the energy equation quickly using a laptop (normally less than 4 CPU hours). However, if the molecular dynamics simulation is used to calculate the temperature, much more time and computational resources are needed, i.e., we consumed around 8000 CPU hours to calculate one case where 1664021 atoms are confined in a channel whose height is 24 nm. However, the analytical solution and numerical modelling based on the continuity assumption also have some limitations. For example, (1) the first order velocity and temperature slip boundary conditions in continuum-based analytical solution and modelling contains constant momentum and thermal accommodation coefficients, which, unfortunately, strongly depend on materials of fluids and the wall, local pressure, velocity and the mean direction of the local flow ([Karniadakis et al., 2006](#)); (2) the density layering and non-uniform viscosity near the interface between the fluid and wall are not considered. For the molecular dynamics (MD) simulation, it has become an effective alternation to study the nanoscale fluid and heat transfer characteristics as it does not introduce any postulation except the potential functions describing the interforce of particles, and it has been used successfully to calculate the transport parameters (i.e., thermal conductivity). Hence, to balance the computational accuracy and time consumption, micro- and nano-scale flow and heat are investigated by the analytical solution, numerical simulation and molecular dynamics simulation in this work.

The overall aim of the thesis is to investigate micro- and nano-scale flow and heat transfer in a channel with phase change. The main objectives are:

1. Studying the effects of axial conduction, viscous dissipation and rar-

efied flow on heat transfer by solving the continuum-based energy equation with the slip boundary conditions.

2. Exploring the resistance loss of the slip flow.
3. Applying the molecular dynamics (MD) simulation to investigate the slip length, and revealing other features of micro- and nano-scale fluid (i.e., non-uniform density and viscosity profiles).
4. Performing the MD simulation to reveal the feature of micro- and nano-scale fluid with phase change (i.e., the thermal de-icing).

The rest of the thesis is organized as follows. In Section 2.1, by using the convective heat transfer featuring the velocity slip and temperature jump in a micro- and nano-scale channel as an example, the continuum-based energy governing equation is analytically solved, and the effects of axial conduction, viscous dissipation and rarefied flow on heat transfer are analyzed. In Section 2.2, the linear Navier velocity slip boundary condition is implemented using three schemes, and the second law analysis (SLA) based on the local entropy generation rate is proposed to compute and visualize the flow resistance in mass transfer through pipe/channel with a sudden contraction component (SCC) at low Reynolds number (Re) featuring velocity slip.

In Chapter 3, molecular dynamics (MD) simulations are conducted to investigate the heat transfer of liquid argon flow through a nanoscale channel, and the nanoscale features (i.e., velocity slip, temperature jump, non-uniform density and viscosity profiles) are revealed.

In Section 4.1, molecular dynamics (MD) simulations are conducted to investigate the underpinning physics of thermal de-icing on a flat wall from the molecular level, and the effects of ice thickness, wall temperature and

wettability on the thermal de-icing process are examined. In Section 4.2, the graphene and carbon nanotubes junction (G-CNTs) is proposed for the first time to be sandwiched between the ice and the hydrophobic (i.e., silicon) and hydrophilic (i.e., silver and copper) substrates, and then molecular dynamics (MD) simulations are performed to investigate the underpinning physics of ice adhesion from the molecular level.

Finally, the main conclusions of the thesis are summarised, and suggestions for future work are illustrated in Chapter 5.

Chapter 2

Heat transfer and flow characteristics of micro-scale flow

In this chapter, convective heat transfer and resistance of micro-scale slip flow are investigated by solving the analytical solution of the energy equation and performing numerical simulations, respectively.

Unlike previous works reviewed in Section 1.2, viscous dissipation term and axial conduction term are considered simultaneously in the process of deriving the analytical solution of the 2D energy equation with the first-order velocity slip model and the temperature jump boundary model. An analytical expression of dimensionless 2D temperature profile via much simpler separation of variables and substitution approaches is obtained, and then it is applied to examine the impacts of viscous dissipation, axial conduction and rarefied effect on heat transfer.

Moreover, to quantitatively examine the flow resistance coefficient and re-

veal the physics in slip flow, a linear Navier velocity slip boundary condition (SBC) is implemented based on the OpenFOAM. Then, the flow resistance coefficients of flow in a plane parallel channel with/without an sudden contraction component and a pipe are determined from the view of exact solutions of the NS and SLA approaches as introduced in Section 1.1.

2.1 An analytical solution of convective heat transfer in microchannel

2.1.1 Energy equation and boundary conditions

The geometry of the parallel plate microchannel or nanochannel is shown in Fig. 2.1.

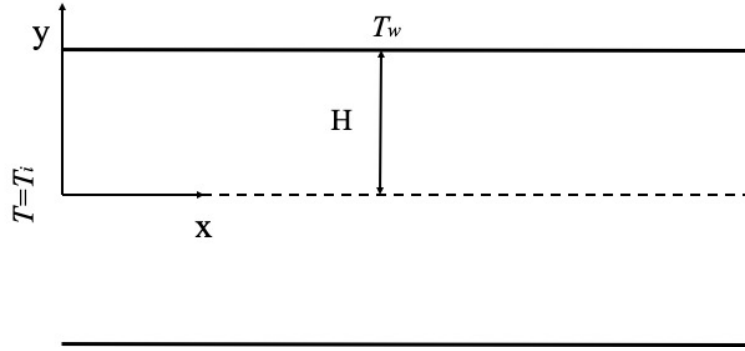


Figure 2.1: Definition sketch.

We assume that (1) the continuum assumption is valid, (2) the flow is incompressible and fully developed, (3) the flow and heat transfer is a 2D problem, (4) fluid property including density, specific heat, thermal conductivity and dynamic viscosity, are constants. Then, flow and heat transfer including axial conduction and viscous dissipation in the aforementioned microchannel or nanochannel is governed by the 2D energy equation and

boundary conditions

$$\rho c_p u \frac{\partial T}{\partial x} = k \frac{\partial^2 T}{\partial x^2} + k \frac{\partial^2 T}{\partial y^2} + \mu \left(\frac{\partial u}{\partial y} \right)^2, \quad (2.1)$$

$$T = T_i \quad \text{at} \quad x = 0, \quad (2.2a)$$

$$\frac{\partial T}{\partial y} = 0 \quad \text{at} \quad y = 0, \quad (2.2b)$$

$$T - T_w = -\frac{2 - \sigma_T}{\sigma_T} \frac{2\gamma}{\gamma + 1} \frac{\lambda}{Pr} \frac{\partial T}{\partial y} \quad \text{at} \quad y = H. \quad (2.2c)$$

In Eq. (2.1), $\rho c_p u \frac{\partial T}{\partial x}$ is the convective term, and the three terms on the right side represent axial conduction, heat conduction normal to the wall and viscous dissipation, respectively. The first and second boundary condition in Eq. (2.2a) and Eq. (2.2b) are the uniform temperature at the channel entrance and symmetry temperature at the centreline, respectively. The third boundary condition shown in Eq. (2.2c) is the first-order temperature jump model (the first-order means that the slip velocity/temperature is proportional to the gradient of velocity/temperature along the wall-normal direction) derived from an energy balance at the wall by Kennard (Kennard, 1962).

2.1.2 Analytical solution of the 2D energy equation

The flow chart of the analytical solution is shown in Fig. 2.2. To solve the energy equation, we define the following dimensionless variables

$$\begin{aligned} \theta &= \frac{T - T_w}{T_i - T_w}, & Br &= \frac{\mu u_{ave}^2}{k(T_i - T_w)}, \\ \xi &= \frac{x}{Re \cdot Pr \cdot H}, & \eta &= \frac{y}{H}. \end{aligned} \quad (2.3)$$

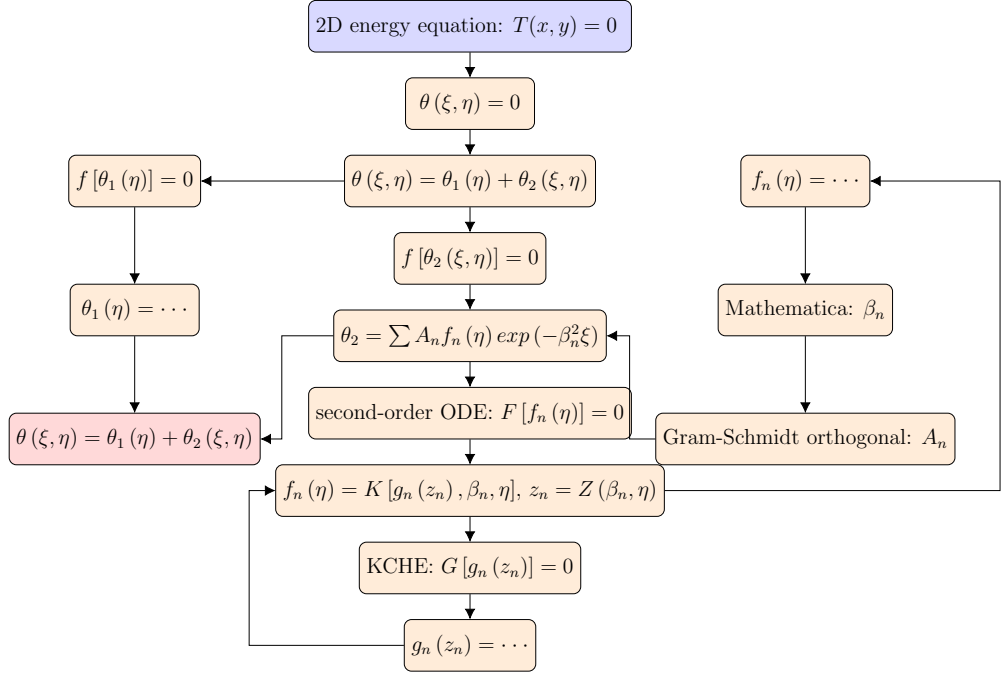


Figure 2.2: Flow chart of the analytical solution of the 2D energy equation (KCHE stands for the Kummer confluent hypergeometric equation).

The energy equation and boundary conditions can thus be non-dimensionalized as

$$\frac{1}{4}u^* \frac{\partial \theta}{\partial \xi} = \frac{1}{Pe^2} \frac{\partial^2 \theta}{\partial \xi^2} + \frac{\partial^2 \theta}{\partial \eta^2} + Br \left(\frac{\partial u^*}{\partial \eta} \right)^2, \quad (2.4)$$

$$\theta = 1 \quad \text{at} \quad \xi = 0, \quad (2.5a)$$

$$\frac{\partial \theta}{\partial \eta} = 0 \quad \text{at} \quad \eta = 0, \quad (2.5b)$$

$$\theta = -4C_1 \frac{\partial \theta}{\partial \eta} \quad \text{at} \quad \eta = 1, \quad (2.5c)$$

where the non-dimensional velocity u^* is given by (Jeong and Jeong, 2006)

$$u^* = \frac{u}{u_{ave}} = \frac{3}{2} \frac{1 - \eta^2 + 8 \frac{2-\sigma}{\sigma} Kn}{C_2}. \quad (2.6)$$

θ can be decomposed as an asymptotic temperature $\theta_1(\xi \rightarrow +\infty)$ and a

transient term

$$\theta = \theta_1 + \theta_2. \quad (2.7)$$

When $\xi \rightarrow +\infty$, there is

$$\frac{\partial \theta_1}{\partial \xi} = 0, \quad \frac{\partial^2 \theta_1}{\partial \xi^2} = 0. \quad (2.8)$$

Subsequently, after substituting Eq. (2.7) and Eq. (2.8) into Eq. (2.4) and Eqs. (2.5a) to (2.5c), we obtain two sets of dimensionless energy equations and boundary conditions for θ_1 and θ_2

$$\frac{\partial^2 \theta_1}{\partial \eta^2} = -Br \left(\frac{\partial u^*}{\partial \eta} \right)^2, \quad (2.9)$$

$$\frac{\partial \theta_1}{\partial \eta} = 0 \quad \text{at} \quad \eta = 0, \quad (2.10a)$$

$$\theta_1 = -4C_1 \frac{\partial \theta_1}{\partial \eta} \quad \text{at} \quad \eta = 1, \quad (2.10b)$$

and

$$\frac{1}{4}u^* \frac{\partial \theta_2}{\partial \xi} - \frac{1}{Pe^2} \frac{\partial^2 \theta_2}{\partial \xi^2} - \frac{\partial^2 \theta_2}{\partial \eta^2} = 0, \quad (2.11)$$

$$\frac{\partial \theta_2}{\partial \eta} = 0 \quad \text{at} \quad \eta = 0, \quad (2.12a)$$

$$\theta_2 = -4C_1 \frac{\partial \theta_2}{\partial \eta} \quad \text{at} \quad \eta = 1. \quad (2.12b)$$

Through solving Eq. (2.9) with boundary conditions Eqs. (2.10a) and (2.10b), the asymptotic temperature θ_1 is obtained,

$$\theta_1 = \frac{Br}{C_2^2} \left(\frac{-3}{4}\eta^4 + \frac{3}{4} + 12C_1 \right). \quad (2.13)$$

According to references (Deen, 1998; Larrodé et al., 2000; Horiuchi et al., 2006; Dutta et al., 2006), the solution θ_2 of the homogeneous partial differential Eq. (2.11) can be written as

$$\theta_2 = \sum_{n=1}^{\infty} A_n f_n(\eta) \exp(-\beta_n^2 \xi). \quad (2.14)$$

In this infinite series, each term consists of a magnitude A_n , a function f_n and an exponential term depending on ξ . After substituting Eq. (2.14) into Eq. (2.11), Eq. (2.12a) and Eq. (2.12b), the following equation and boundary conditions can be obtained

$$\frac{d^2 f_n(\eta)}{d\eta^2} + \beta_n^2 \left(\frac{1}{4} u^* + \frac{\beta_n^2}{Pe^2} \right) f_n(\eta) = 0, \quad (2.15)$$

$$\frac{d f_n(\eta)}{d\eta} = 0 \quad \text{at} \quad \eta = 0, \quad (2.16a)$$

$$f_n(\eta) = -4C_1 \frac{d f_n(\eta)}{d\eta} \quad \text{at} \quad \eta = 1, \quad (2.16b)$$

where $f_n(\eta)$ and β_n are eigenfunctions and eigenvalues, respectively.

Now, we define two new variables

$$f_n(\eta) = \exp\left(\frac{-1}{2}\beta_n\sqrt{k_2}\eta^2\right) g_n(z_n), \quad (2.17a)$$

$$z_n = \beta_n\sqrt{k_2}\eta^2. \quad (2.17b)$$

With the dimensionless velocity in Eq. (2.6), boundary condition in Eq. (2.16a) and variable transformation in Eqs. (2.17a) and (2.17b), Eq. (2.15) can be

reformulated as

$$z_n \frac{d^2 g_n(z_n)}{dz_n^2} + \left(\frac{1}{2} - z_n \right) \frac{dg_n(z_n)}{dz_n} - g_n(z_n) \cdot \frac{-\beta_n^3 - k_1 Pe^2 \beta_n - k_2 Pe^2 \beta_n + Pe^2 \sqrt{k_2}}{4Pe^2 \sqrt{k_2}} = 0. \quad (2.18)$$

Eq. (2.18) is the standard confluent hypergeometric equation, whose solution can be expressed as

$$g_n(z_n) = {}_1F_1(a_n, b_n; z_n) = \sum_{m=0}^{\infty} \frac{(a_n)^{(m)} (z_n)^m}{(b_n)^{(m)} m!}, \quad (2.19)$$

where ${}_1F_1(a_n, b_n; z_n)$ is the confluent hypergeometric function (George et al., 2013) and a_n and b_n are

$$a_n = \frac{-\beta_n^3 - k_1 Pe^2 \beta_n - k_2 Pe^2 \beta_n + Pe^2 \sqrt{k_2}}{4Pe^2 \sqrt{k_2}}, \quad (2.20)$$

$$b_n = \frac{1}{2}.$$

After substituting Eq. (2.19) into Eq. (2.17a), the eigenfunctions $f_n(\eta)$ become

$$f_n(\eta) = \exp\left(\frac{-1}{2} \beta_n \sqrt{k_2} \eta^2\right) \sum_{m=0}^{\infty} \frac{(a_n)^{(m)} (z_n)^m}{(b_n)^{(m)} m!}. \quad (2.21)$$

These eigenvalues β_n can be determined via applying the boundary condition in Eq. (2.16b).

Therefore, θ_2 in Eq. (2.14) can be calculated from

$$\theta_2 = \sum_{n=1}^{\infty} A_n \left[\sum_{m=0}^{\infty} \frac{(a_n)^{(m)} (z_n)^m}{(b_n)^{(m)} m!} \exp\left(\frac{-1}{2} \beta_n \sqrt{k_2} \eta^2\right) \right] \cdot \exp(-\beta_n^2 \xi), \quad (2.22)$$

where a_n , b_n , and z_n are shown in Eq. (2.20) and Eq. (2.17b), respectively.

Substituting Eq. (2.22) and Eq. (2.13) into Eq. (2.7), we can obtain

$$\theta = \frac{Br}{C_2^2} \left(\frac{-3}{4} \eta^4 + \frac{3}{4} - 12C_1 \right) + \sum_{n=1}^{\infty} A_n \cdot \left[\sum_{m=0}^{\infty} \frac{(a_n)^{(m)}(z_n)^m}{(b_n)^{(m)}m!} \exp \left(\frac{-1}{2} \beta_n \sqrt{k_2} \eta^2 \right) \right] \exp(-\beta_n^2 \xi). \quad (2.23)$$

The summation constants A_n can be obtained from the boundary condition in Eq. (2.5a) by using the Gram-Schmidt orthogonal approach illustrated in detail in Section 2.1.3 (the algorithm of this method is outlined in Section 2.1.3) or the Least-square method shown in Appendix A.

Once unknown eigenvalues β_n and summation coefficients A_n are determined, we can obtain the dimensionless temperature θ in the microchannel or nanochannel. The dimensionless bulk temperature θ_b (the bulk temperature is that adiabatic mixing of the fluid from a prescribed cross section of the pipe/channel will result in some equilibrium temperature that accurately reflects the average temperature of the moving fluid) for fluid flow through the parallel channel and the local Nusselt number which is the ratio of convective to conductive heat transfer normal to the wall boundary can be calculated from following equations, respectively:

$$\theta_b(\xi) = \int_0^1 u^*(\eta) \theta(\xi, \eta) d\eta, \quad (2.24)$$

$$Nu_L = \frac{hD_H}{k} = -\frac{4}{\theta_b(\xi)} \frac{\partial \theta(\xi, \eta)}{\partial \eta} \bigg|_{\eta=1}. \quad (2.25)$$

The bulk temperature T_b for fluid is

$$\begin{aligned} T_b(x) &= \frac{\int_0^H \rho u(y) W c_p T(x, y) dy}{\int_0^H \rho u(y) W c_p dy} = \frac{\int_0^H u(y) T(x, y) dy}{\int_0^H u(y) dy} \\ &= \frac{1}{Hu_{ave}} \int_0^H u(y) T(x, y) dy = \frac{1}{H} \int_0^H u^*(y) T(x, y) dy. \end{aligned} \quad (2.26)$$

2.1.3 Determination of summation constants

Gram-Schmidt orthogonal approach

Let us assume a series of orthogonal function g_i to make

$$\theta_2 = \sum A_n f_n \exp(-\beta_n^2 \xi) = \sum B_n g_n \exp(-\beta_n^2 \xi), \quad (2.27)$$

where B_n is also the summation coefficient. The relation between g_i and eigenfunction is

$$g_1 = f_1 \quad (2.28a)$$

$$g_2 = f_2 - \alpha_{21} f_1 \quad (2.28b)$$

$$g_3 = f_3 - \alpha_{31} f_1 - \alpha_{32} f_2 \quad (2.28c)$$

$$g_4 = f_4 - \alpha_{41} f_1 - \alpha_{42} f_2 - \alpha_{43} f_3 \quad (2.28d)$$

$$\vdots$$

$$g_N = f_N - \sum_{j=1, N \geq 2}^{N-1} \alpha_{Nj} f_j, \quad (2.28e)$$

where α_{ij} are constants. In the following step, efforts are made to calculate these constants before determining orthogonal functions g_i . For convenience, we apply a symbol $\otimes$ and define

$$\int_0^1 f \cdot g \, d\eta = f \otimes g. \quad (2.29)$$

Now by multiplying Eq. (2.28b) with g_1 and integrating over the domain ($0 \leq \eta \leq 1$) based on the property of orthogonal function, we can obtain

$$g_2 \otimes g_1 = f_2 \otimes g_1 - \alpha_{21} f_1 \otimes g_1 = 0, \quad (2.30)$$

and then α_{21} is

$$\alpha_{21} = \frac{f_2 \otimes g_1}{f_1 \otimes g_1}. \quad (2.31)$$

Then we respectively multiply Eq. (2.28c) with g_1, g_2 and perform integration in domain ($0 \leq \eta \leq 1$)

$$g_3 \otimes g_1 = f_3 \otimes g_1 - \alpha_{31} f_1 \otimes g_1 - \alpha_{32} f_2 \otimes g_1 = 0 \quad (2.32a)$$

$$g_3 \otimes g_2 = f_3 \otimes g_2 - \alpha_{31} f_1 \otimes g_2 - \alpha_{32} f_2 \otimes g_2 = 0 \quad (2.32b)$$

The above Eqs. (2.32a) and (2.32b) can be written as a matrix

$$\begin{bmatrix} f_1 \otimes g_1 & f_2 \otimes g_1 \\ f_1 \otimes g_2 & f_2 \otimes g_2 \end{bmatrix} \begin{bmatrix} \alpha_{31} \\ \alpha_{32} \end{bmatrix} = \begin{bmatrix} f_3 \otimes g_1 \\ f_3 \otimes g_2 \end{bmatrix}. \quad (2.33)$$

Similarly, we can also multiply respectively Eq. (2.28d) with g_1, g_2 and g_3 , and Eq. (2.28e) with $g_1, g_2, \dots, g_{N-1}$, integrate all terms in these equations

over the zone ($0 \leq \eta \leq 1$) and rearrange these into matrix form

$$\begin{bmatrix} f_1 \otimes g_1 & f_2 \otimes g_1 & f_3 \otimes g_1 \\ f_1 \otimes g_2 & f_2 \otimes g_2 & f_3 \otimes g_2 \\ f_1 \otimes g_3 & f_2 \otimes g_3 & f_3 \otimes g_3 \end{bmatrix} \begin{bmatrix} \alpha_{41} \\ \alpha_{42} \\ \alpha_{43} \end{bmatrix} = \begin{bmatrix} f_4 \otimes g_1 \\ f_4 \otimes g_2 \\ f_4 \otimes g_3 \end{bmatrix} \quad (2.34a)$$

$$\begin{aligned} & \vdots \\ & \begin{bmatrix} f_1 \otimes g_1 & f_2 \otimes g_1 & \cdots & f_{N-1} \otimes g_1 \\ f_1 \otimes g_2 & f_2 \otimes g_2 & \cdots & f_{N-1} \otimes g_2 \\ \vdots & \vdots & \vdots & \vdots \\ f_1 \otimes g_{N-1} & f_2 \otimes g_{N-1} & \cdots & f_{N-1} \otimes g_{N-1} \end{bmatrix} \\ & \begin{bmatrix} \alpha_{N1} \\ \alpha_{N2} \\ \vdots \\ \alpha_{NN-1} \end{bmatrix} = \begin{bmatrix} f_N \otimes g_1 \\ f_N \otimes g_2 \\ \vdots \\ f_N \otimes g_{N-1} \end{bmatrix}. \end{aligned} \quad (2.34b)$$

In addition to that, according to Eqs. (2.28a) to (2.28e) and property of orthogonal function, we can get

$$f_m \otimes g_n = 0, \quad \text{if} \quad (m < n). \quad (2.35)$$

Hence, Eqs. (2.33), (2.34a) and (2.34b) could be simplified to

$$\begin{bmatrix} f_1 \otimes g_1 & f_2 \otimes g_1 \\ 0 & f_2 \otimes g_2 \end{bmatrix} \begin{bmatrix} \alpha_{31} \\ \alpha_{32} \end{bmatrix} = \begin{bmatrix} f_3 \otimes g_1 \\ f_3 \otimes g_2 \end{bmatrix}, \quad (2.36a)$$

$$\begin{bmatrix} f_1 \otimes g_1 & f_2 \otimes g_1 & f_3 \otimes g_1 \\ 0 & f_2 \otimes g_2 & f_3 \otimes g_2 \\ 0 & 0 & f_3 \otimes g_3 \end{bmatrix} \begin{bmatrix} \alpha_{41} \\ \alpha_{42} \\ \alpha_{43} \end{bmatrix} = \begin{bmatrix} f_4 \otimes g_1 \\ f_4 \otimes g_2 \\ f_4 \otimes g_3 \end{bmatrix} \quad (2.36b)$$

$$\begin{bmatrix} f_1 \otimes g_1 & f_2 \otimes g_1 & \cdots & f_{N-1} \otimes g_1 \\ 0 & f_2 \otimes g_2 & \cdots & f_{N-1} \otimes g_2 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & f_{N-1} \otimes g_{N-1} \end{bmatrix} \begin{bmatrix} \alpha_{N1} \\ \alpha_{N2} \\ \vdots \\ \alpha_{NN-1} \end{bmatrix} = \begin{bmatrix} f_N \otimes g_1 \\ f_N \otimes g_2 \\ \vdots \\ f_N \otimes g_{N-1} \end{bmatrix}. \quad (2.36c)$$

These above equations can be simply written as a matrix equation

$$\mathbf{L} \cdot \mathbf{V} = \mathbf{R}. \quad (2.37)$$

From Eqs. (2.28a) to (2.28e) and (2.36a) to (2.36c), all coefficients α_{nm} and orthogonal functions g_i could be obtained. In the following section, we will make effort to determine coefficients B_n from initial boundary condition $\xi = 0, \theta = 1$. Based on $\theta = \theta_1 + \theta_2$ and the boundary condition, we can get

$$\begin{aligned} \theta &= \theta_1 + \theta_2 = \theta_1 + \sum A_n f_n \exp(-\beta_n^2 \xi) \\ &= \theta_1 + \sum B_n g_n \exp(-\beta_n^2 \xi) = 1. \end{aligned} \quad (2.38)$$

Multiply Eq. (2.38) with g_n and conducting integration in zone $[0, 1]$ and then coefficients B_n may be calculated from

$$B_n = \frac{(1 - \theta_1) \otimes g_n}{g_n \otimes g_n}. \quad (2.39)$$

When $\xi = 0$, the Eq. (2.27) is transformed into

$$\sum A_n f_n = \sum B_n g_n. \quad (2.40)$$

Then, Eqs. (2.28a) to (2.28e) are substituted in Eq. (2.40)

$$\begin{aligned} \sum A_n f_n &= \sum B_n g_n \\ &= B_1 g_1 + B_2 g_2 + B_3 g_3 + B_4 g_4 + \cdots + B_N g_N \\ &= B_1 f_1 + B_2 (f_2 - \alpha_{21} f_1) + B_3 (f_3 - \alpha_{31} f_1 - \alpha_{32} f_2) \\ &\quad + B_4 (f_4 - \alpha_{41} f_1 - \alpha_{42} f_2 - \alpha_{43} f_3) \\ &\quad + \cdots \\ &\quad + B_N \left(f_N - \sum_{j=1, N \geq 2}^{N-1} \alpha_{Nj} f_j \right) \\ &= (B_1 - \alpha_{21} B_2 - \alpha_{31} B_3 - \alpha_{41} B_4 - \cdots - \alpha_{N1} B_N) f_1 \\ &\quad + (B_2 - \alpha_{32} B_3 - \alpha_{42} B_4 - \cdots - \alpha_{N2} B_N) f_2 \\ &\quad + (B_3 - \alpha_{43} B_4 - \cdots - \alpha_{N3} B_N) f_3 \\ &\quad + (B_4 - \cdots - \alpha_{N4} B_N) f_4 \\ &\quad + \cdots \\ &\quad + B_N f_N. \end{aligned} \quad (2.41)$$

Hence, coefficients A_n become

$$\begin{aligned}
 A_1 &= B_1 - \alpha_{21}B_2 - \alpha_{31}B_3 - \alpha_{41}B_4 - \cdots - \alpha_{N1}B_N \\
 A_2 &= B_2 - \alpha_{32}B_3 - \alpha_{42}B_4 - \cdots - \alpha_{N2}B_N \\
 A_3 &= B_3 - \alpha_{43}B_4 - \cdots - \alpha_{N3}B_N \\
 A_4 &= B_4 - \cdots - \alpha_{N4}B_N \\
 &\vdots \\
 A_N &= B_N.
 \end{aligned} \tag{2.42}$$

That is

$$\begin{aligned}
 A_n &= B_n - \sum_{m=n+1}^N \alpha_{mn}B_m \quad \text{at } 1 \leq n \leq N-1 \\
 A_N &= B_N.
 \end{aligned} \tag{2.43}$$

The algorithm about applying the Gram-Schmidt orthogonal approach to determine summation constants

Start of the algorithm determining coefficients A_n by applying Gram-Schmidt orthogonal procedure.

1. Determine eigenvalues β_n ($1 \leq n \leq N$) from the boundary condition in Eq. (2.16b). N is the number of eigenvalues or eigenfunctions.
2. Define a user function that can integrate the product of two arbitrary functions over the arbitrary domain $[a, b]$ ($a < b$) by using the Gauss-Legendre quadrature method as this method can calculate numerical integration with high accuracy and short CPU times.
3. Input β_n , Pe , a_n , b_n , N to obtain $f_n(\eta)$.
4. Calculate g_1 on the basis of Eq. (2.28a), α_{21} from on the basis of

Eq. (2.31) and g_2 based on Eq. (2.28b) respectively. Store g_1 and g_2 into a list named g .

5. Set an index number $p=3$.
6. Apply the user definition integration function in Step 2 to determine the left matrix $\mathbf{L}$, the right matrix $\mathbf{R}$ and vector $\mathbf{V}$ in Eq. (2.37) and g_p . Store g_p in a list g and set $p = p + 1$.
7. Compare the p and N
 - if ($p \leq N$)
 - go to Step 6.
 - else
 - move to the next step.
8. Calculate coefficients B_n based on boundary condition.
9. Determine coefficients A_n from Eq. (2.43).

End of the algorithm.

For example, Table 2.1 and Table 2.2 show the first 20 eigenvalues and summation coefficients determined via using the Gram-Schmidt orthogonal approach at various Knudsen number and Brinkman number.

2.1.4 Validation of the analytical solution

The infinite series in Eq. (2.22) can be truncated to the first N terms to approximate the non-dimensional temperature θ_2 with the reduced computational cost. At $N = 20$, the dimensionless bulk temperature can be converged to 5 significant figures. Then $N = 20$ is used in the following sections, the same as adopted in references (Barışık et al., 2015; Dutta et al., 2006).

2.1. AN ANALYTICAL SOLUTION OF CONVECTIVE HEAT TRANSFER IN MICROCHANNEL

Table 2.1: First 20 eigenvalues and coefficients for $Pe = 10^6$, $Br = 0.00$

n	Kn=0.00		Kn=0.04		Kn=0.08	
	β_n	A_n	β_n	A_n	β_n	A_n
1	2.7460	1.2010	2.3336	1.1768	2.0341	1.1481
2	9.2588	-0.2997	8.1700	-0.2517	7.5513	-0.2007
3	15.7882	0.1616	14.1779	0.1160	13.4858	0.0781
4	22.3192	-0.1085	20.2895	-0.0667	19.6004	-0.0401
5	28.8507	0.0810	26.4707	0.0431	25.7994	0.0241
6	35.3824	-0.0644	32.6992	-0.0299	32.0425	-0.0159
7	41.9142	0.0535	38.9603	0.0219	38.3110	0.0113
8	48.4460	-0.0458	45.2446	-0.0167	44.5954	-0.0084
9	54.9779	0.0401	51.5457	0.0131	50.8901	0.0065
10	61.5098	-0.0359	57.8592	-0.0106	57.1921	-0.0052
11	68.0417	0.0326	64.1822	0.0087	63.4994	0.0042
12	74.5737	-0.0301	70.5125	-0.0073	69.8104	-0.0035
13	81.1056	0.0282	76.8486	0.0062	76.1244	0.0030
14	87.6376	-0.0268	83.1893	-0.0054	82.4407	-0.0025
15	94.1695	0.0258	89.5338	0.0047	88.7588	0.0022
16	100.7015	-0.0253	95.8814	-0.0042	95.0784	-0.0019
17	107.2334	0.0254	102.2315	0.0038	101.3991	0.0017
18	113.7654	-0.0263	108.5839	-0.0035	107.7208	-0.0016
19	120.2973	0.0290	114.9380	0.0034	114.0434	0.0015
20	126.8293	-0.0380	121.2937	-0.0037	120.3667	-0.0015

Then, we compare our results with those of Jeong et al. (Jeong and Jeong, 2006) to validate the accuracy of our non-dimensional analytical solution of the energy equation. After substituting the first 20 eigenvalues and summation coefficients determined via using the Gram-Schmidt orthogonal approach (see Appendix 2.1.3) into Eq. (2.25) and Eq. (2.24), the rarefied effect on local Nusselt and how viscous dissipation affects the fluid bulk temperature distribution are shown in Fig. 2.3 and Fig. 2.4, respectively. It can be seen that our results are in excellent agreement with the reference (Jeong and Jeong, 2006).

In addition to that, we also redefine non-dimensional variables and re-address the dimensionless energy equation in literature (Barışık et al., 2015). The asymptotic Nusselt number at $\widetilde{Pe} = 1.0, Kn = 0, Br = 0$ computed using the present approach is 4.0273, which is nearly equal to 4.027 from the reference (Barışık et al., 2015).

Besides, the temperature and velocity slip boundary conditions shown in Eq. (2.2c) and Eq. (2.6) are implemented based on the OpenFOAM. Then,

2.1. AN ANALYTICAL SOLUTION OF CONVECTIVE HEAT TRANSFER IN MICROCHANNEL

Table 2.2: First 20 eigenvalues and coefficients for $Pe = 10^6$, $Kn = 0.00$

n	Br=0.0		Br=0.2		Br=-0.2	
	β_n	A_n	β_n	A_n	β_n	A_n
1	2.7460	1.2010	2.7460	1.0285	2.7460	1.3735
2	9.2588	-0.2997	9.2588	-0.2710	9.2588	-0.3283
3	15.7882	0.1616	15.7882	0.1529	15.7882	0.1704
4	22.3192	-0.1085	22.3192	-0.1046	22.3192	-0.1124
5	28.8507	0.0810	28.8507	0.0789	28.8507	0.0832
6	35.3824	-0.0644	35.3824	-0.0631	35.3824	-0.0658
7	41.9142	0.0535	41.9142	0.0526	41.9142	0.0544
8	48.4460	-0.0458	48.4460	-0.0452	48.4460	-0.0464
9	54.9779	0.0401	54.9779	0.0397	54.9779	0.0406
10	61.5098	-0.0359	61.5098	-0.0355	61.5098	-0.0362
11	68.0417	0.0326	68.0417	0.0324	68.0417	0.0329
12	74.5737	-0.0301	74.5737	-0.0299	74.5737	-0.0303
13	81.1056	0.0282	81.1056	0.0280	81.1056	0.0284
14	87.6376	-0.0268	87.6376	-0.0266	87.6376	-0.0269
15	94.1695	0.0258	94.1695	0.0257	94.1695	0.0259
16	100.7015	-0.0253	100.7015	-0.0252	100.7015	-0.0254
17	107.2334	0.0254	107.2334	0.0253	107.2334	0.0255
18	113.7654	-0.0263	113.7654	-0.0262	113.7654	-0.0264
19	120.2973	0.0290	120.2973	0.0289	120.2973	0.0291
20	126.8293	-0.0380	126.8293	-0.0378	126.8293	-0.0381

a case is tested by the open-source code and the aforementioned analytical solution, and the outcome is shown in Fig. 2.5. One can observe that the dimensionless bulk temperature computed from these two methods coincide with other.

All comparisons, therefore, indicate that our non-dimensional analytical solution has sufficient accuracy. In the following section, this approach is utilized to analyze how viscous dissipation, axial conduction and rarefied affect heat transfer characteristics.

2.1.5 Results on the overshoot of fluid temperature

The key finding of the present work is that the fluid bulk temperature reaches a value higher than the constant wall temperature, even when the fluid at the inlet is cooler than the wall, as shown in Fig. 2.6. This value is constant at a given set of Pe , Br and Kn , which represent the viscous dissipation, axial condition and rarified effects.

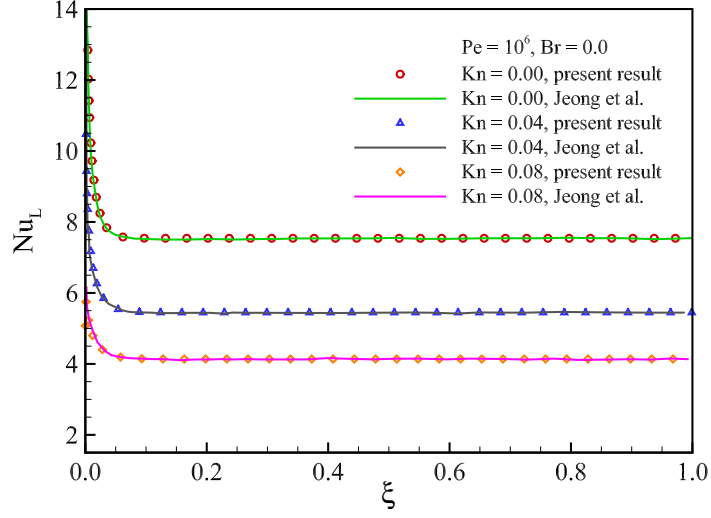


Figure 2.3: Effects of rarefied on local Nusselt number when axial conduction and viscous dissipation are neglected.

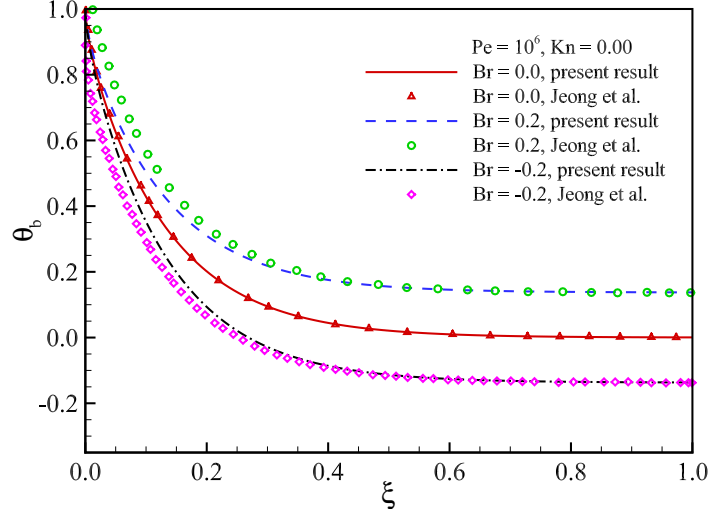


Figure 2.4: Viscous dissipation effects on fluid bulk temperature.

To detailedly illustrate this convergence development of the fluid bulk temperature at various inlet conditions, we test the developments of T_b at various viscous conditions represented by $|Br|$, as shown in Fig. 2.7. The rarefied effect and axial conduction are excluded by setting $Kn = 0$ and $Pe = 10^6$, as will be explained later in the following sections. $Br > 0$ and $Br < 0$ correspond to the cases where the fluid inlet temperature is higher and lower than the constant wall temperature, respectively, as defined in Eq. (2.3). For both cases, the asymptotic dimensionless fluid temperature converges to the same value θ_{bF} ($\theta_{bF} = \frac{T_{bF} - T_w}{T_i - T_w}$). This result is robust even

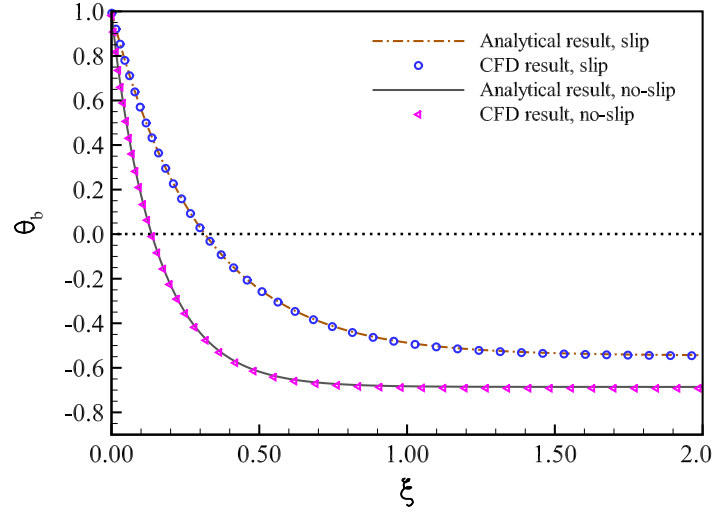


Figure 2.5: Dimensionless bulk temperature profile obtained from CFD simulations and analytical solutions at $Pe = 10$, $Br = -1$, $Kn = 0.1$.

when the initial conditions (ΔT and $\Delta T'$ in Fig. 2.7) are varied. A similar temperature overshoot without an exact value was reported before in separated cooling and heating tests (Hetsroni et al., 2005a; Yarin et al., 2008). In the present study, it is clarified that, because viscous dissipation generates an additional amount of heat, the asymptotic temperature of the fluid is always higher than the constant wall temperature, regardless of the inlet condition of the fluid. Further, the exact temperature overshoot and its dependence on Pe , Br and Kn are obtained. In addition, care must be taken that there is a critical point denoted as ξ_c in Fig. 2.7 as reported in literatures (Nield et al., 2003; Tiselj et al., 2004; Hetsroni et al., 2005b). The fluid bulk temperature is equal to the wall temperature at this point for $Br < 0$ cases. Clearly, ξ_c can be interpreted as the effective length of the channel for cooling. It is also seen in the figure that a higher temperature overshoot corresponds to a lower length of the channel for effective cooling.

Then we turn to the development of the fluid non-dimensional bulk temperature at more general conditions. Fig. 2.8 shows the profile of the bulk temperature at various viscous and rarified conditions, while the axial con-

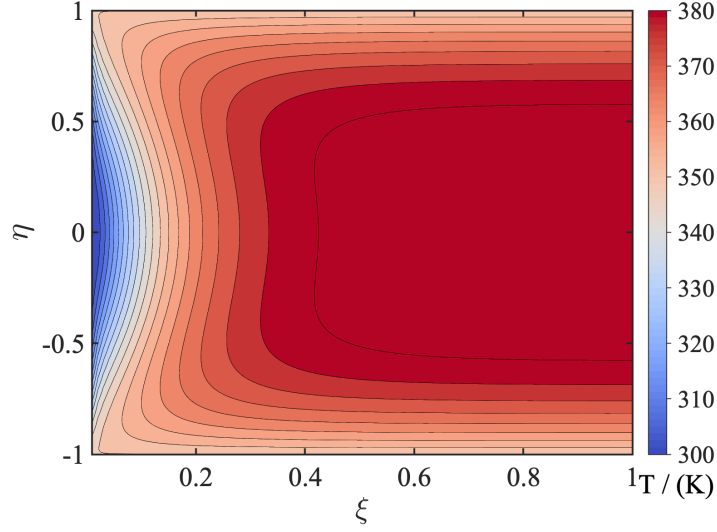


Figure 2.6: The contour of temperature in the 2D channel at $Pe = 10^6$, $Kn = 0.00$, $Br = -1.0$ (The inlet temperature of the fluid and the wall temperature are 300 K and 350 K, respectively).

duction is still neglected by setting $Pe = 10^6$. At $Br = 0$, where there is no viscous dissipation, $\theta_{bF} = 0$ for all the cases considered. With increasing Br , θ_{bF} increases almost linearly for all Kn considered. Also, θ_{bF} roughly reduces at higher Kn . Here Kn quantifies the rarified effects as will be shown later and as it increases, the fluid flow moves from the continuous flow regime ($Kn = 0$ corresponds to the continuum flow regime as reported by (Kandlikar et al., 2005)) to the slip-flow regime (see Fig. 2.8). Similar results (not shown here) have been observed for $Pe = 10$, where the axial conduction effect is activated.

These observations indicate that the magnitude of the overshooting fluid dimensionless bulk temperature is a linear function of Br , and it vanishes when the viscous dissipation is neglected. This overshoot reduces with Kn , the rarified effect, but is insensitive to Pe , the axial conduction effect.

The critical point ξ_c observed in Fig. 2.7, at which the temperature of fluids is equal to the wall temperature, deserves further studies and the variation of ξ_c with respect to Br , Pe and Kn is investigated. In Fig. 2.9a, 36 cases

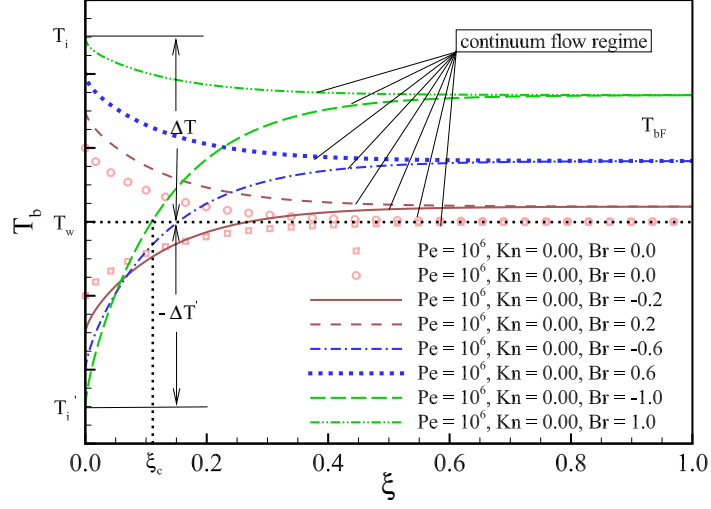


Figure 2.7: Fluid dimensionless bulk temperature profile.

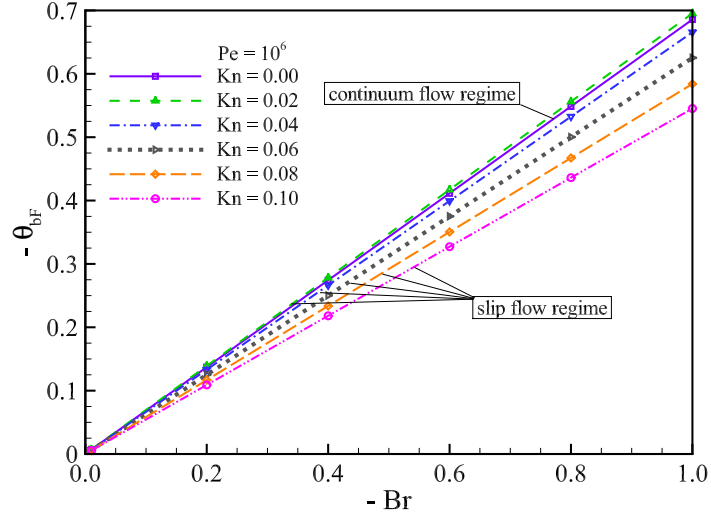


Figure 2.8: Fluid asymptotic dimensionless bulk temperature profile when neglecting axial conduction.

(considering six values of Kn and six values of Br at each Kn) are studied to reveal effects of Kn and Br on ξ_c when neglecting axial conduction by setting $Pe = 10^6$, and then 45 cases including five values of Kn and Br (nine values of Pe at each group of Kn and Br) are conducted to further examine how Pe affects ξ_c in Fig. 2.9b. Clearly, ξ_c reduces with larger Br and Pe and smaller Kn , corresponding to stronger viscous dissipation, weaker axial conduction and weaker rarified effect, respectively.

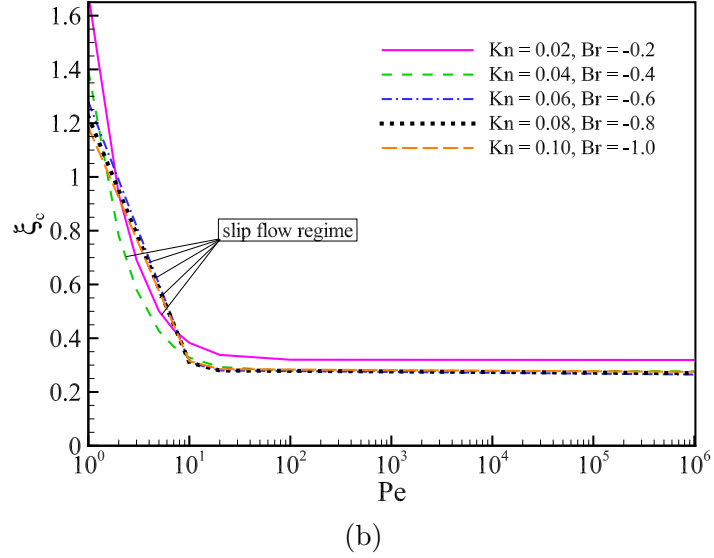
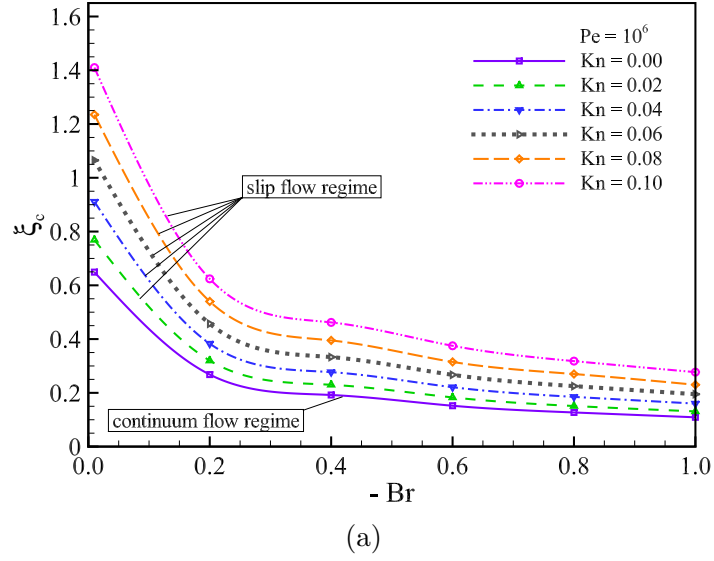


Figure 2.9: Distribution of the critical length ξ_c . (a) ξ_c changes with Br and Kn when neglecting axial conduction. (b) ξ_c profile at different Pe .

2.1.6 Parameter dependence of the heat transfer

It has been shown that three parameters Kn , Pe and Br have critical roles in the temperature overshoot. Each of them will be studied individually in this section to illustrate their effects on the heat transfer between the fluid and the channel, quantified by the local and asymptotic Nusselt number, dimensionless temperature jump and non-dimensional bulk temperature profiles.

Effect of viscous dissipation

The effect of Br on Nu_L when neglecting the rarefied effect and axial conduction is illustrated in Fig. 2.10. Based on Eq. (2.3), $Br > 0$ and $Br < 0$ mean that the inlet temperature of the fluid is higher or lower than the uniform wall temperature, respectively. $Br = 0$ indicates that the viscous dissipation is not taken into consideration. It can be seen from the figure that if neglecting Kn and Pe effects the asymptotic Nusselt number with or without viscous dissipation is 17.5 or 7.54 (the latter value is in agreement with previous studies (Jeong and Jeong, 2006; Ge et al., 2015), which further validates the present analytical solution approach of the 2D energy equation), respectively. Clearly, these values suggest that $Br = 0$ is a singular point where the change of Nusselt number is discontinuous. This singularity can be validated analytically. After substituting Eq. (2.7) and Eq. (2.24) into Eq. (2.25), Nu_L can be written as

$$Nu_L = \frac{-4 \left[\left. \frac{\partial \theta_1(\eta)}{\partial \eta} \right|_{\eta=1} + \left. \frac{\partial \theta_2(\xi, \eta)}{\partial \eta} \right|_{\eta=1} \right]}{\int_0^1 u^*(\eta) [\theta_1(\eta) + \theta_2(\xi, \eta)] d\eta}, \quad (2.44)$$

where θ_1 and θ_2 are shown in Eq. (2.13) and Eq. (2.22), respectively. For all cases mentioned in this sub-section, Nu_L is

$$Nu_L = \frac{-4 \left[-3Br + \left. \frac{\partial \theta_2(\xi, \eta)}{\partial \eta} \right|_{\eta=1} \right]}{\frac{24}{35}Br + \int_0^1 u^*(\eta) \theta_2(\xi, \eta) d\eta}. \quad (2.45)$$

When $Br \neq 0$ and $\xi \rightarrow +\infty$, $\theta_2(\xi, \eta)$ tends to 0. Hence, the asymptotic Nusselt number is

$$Nu_F = \frac{12Br}{\frac{24}{35}Br} = 17.5. \quad (2.46)$$

Obviously, if $Br = 0$, we have

$$Nu_F = \lim_{\xi \rightarrow +\infty} \left[\frac{-4 \frac{\partial \theta_2(\xi, \eta)}{\partial \eta} \Big|_{\eta=1}}{\int_0^1 u^*(\eta) \theta_2(\xi, \eta) d\eta} \right] = 7.54. \quad (2.47)$$

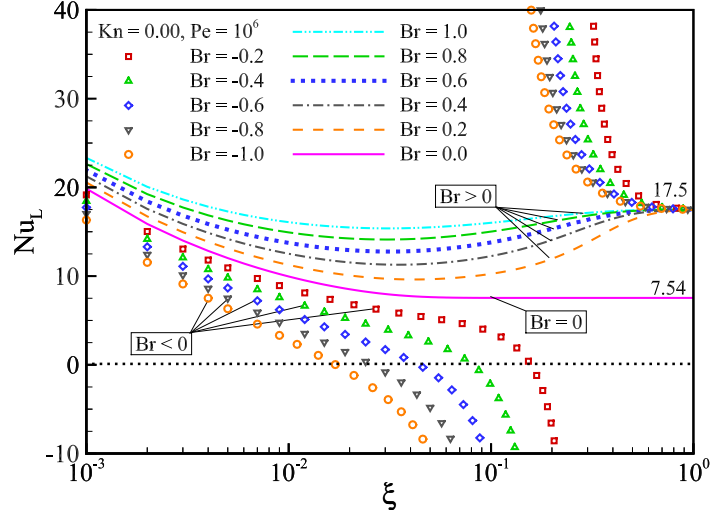


Figure 2.10: Viscous dissipation effect on local Nusselt number.

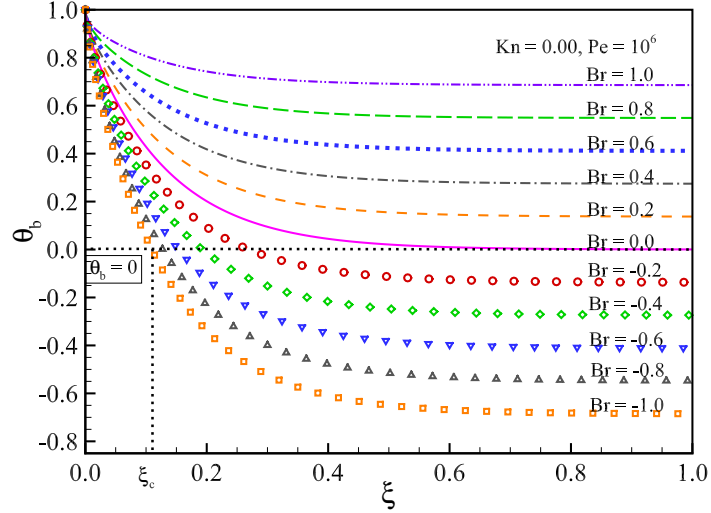


Figure 2.11: Viscous dissipation effect on bulk dimensionless temperature.

Moreover, it is worth noting that $Br < 0$ induces a singular point where Nu_L approximates infinity. This is caused by the definition of the Nusselt number ($Nu_L = -\frac{4}{\theta_b(\xi)} \frac{\partial \theta(\xi, \eta)}{\partial \eta} \Big|_{\eta=1}$). There is a point where the dimensionless bulk temperature of fluid is equal to wall temperature (so θ_b is equal to 0.) as can be found in Fig. 2.11.

The bulk dimensionless temperature profiles at various Br number without Pe and Kn effect are described in Fig. 2.11. The difference between asymptotic fluid bulk temperature and inlet temperature of fluid increases with a reduction in Br if $Br > 0$. The asymptotic fluid temperature equals to wall temperature for $Br = 0$ corresponding to neglecting viscous dissipation. As mentioned in Section 2.1.5 for $Br < 0$ cases, it can be still observed that there is a critical point ξ_c . θ_b equal to 0 at this point, which means the fluid temperature equal to the wall temperature. For $\xi > \xi_c$, θ_b will be less than 0, suggesting that the fluid temperature exceeds the wall temperature, and the effective cooling length is reduced with an increase in $|Br|$. These observations indicate that the cooling effect will be over-estimated when neglecting viscous dissipation.

Effect of axial conduction

It is well known that axial conduction can rise in instances of small Re and Pr since thermal diffusion becomes more important than advection. The dimensionless Pe is usually applied to characterize the effect of axial conduction. As discussed in the introduction, there has been no consensus on the impact of axial conduction on heat transfer. Hence, nine cases ($Pe = 1, Pe = 2, Pe = 3, Pe = 5, Pe = 7, Pe = 10, Pe = 20, Pe = 100, Pe = 10^6$) are performed to clarify its influence.

As shown in Fig. 2.12a, local Nusselt numbers for nine cases converge to various asymptotic values when neglecting the rarefied effect and viscous dissipation. However, for $Pe = 1$ or below, Nu is much larger than other cases especially in the thermal developing region. δ_{Nu} (defined as the relative difference of Nu_L , $\delta_{Nu} = \frac{Nu_L - Nu_L|_{Pe=10^6}}{Nu_L|_{Pe=10^6}} \times 100\%$) decreases rapidly and then maintains a constant level along the flow direction. The value

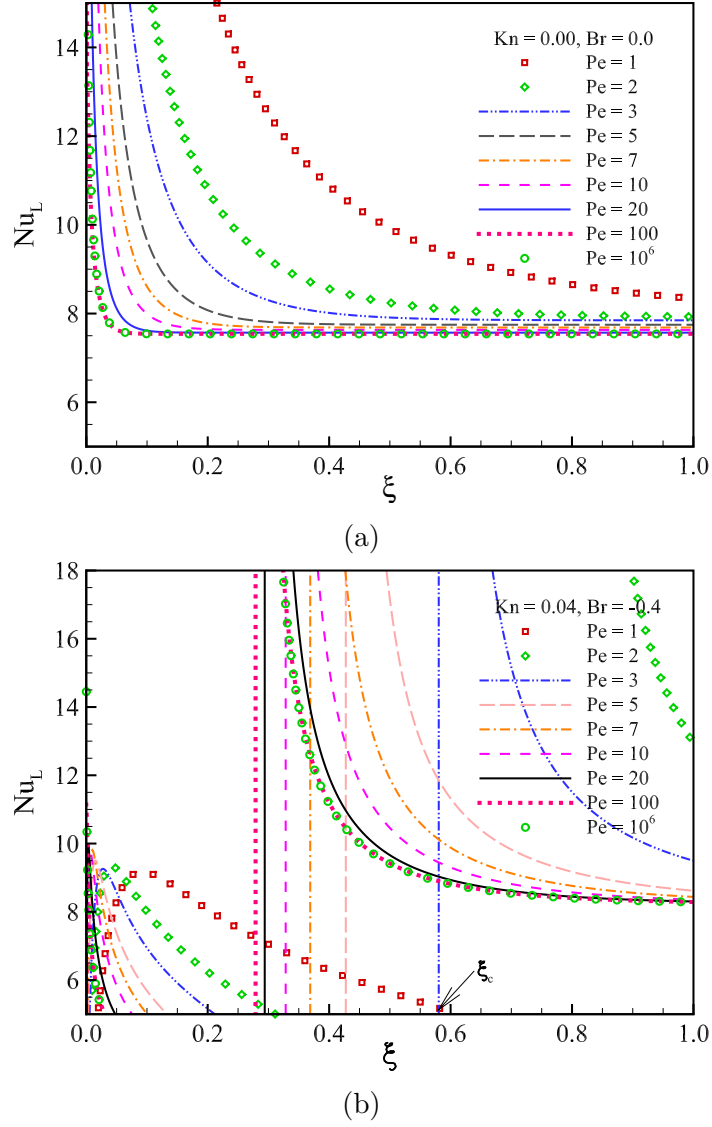


Figure 2.12: Local Nusselt number at various Pe number when considering rarefied effects and viscous dissipation (a) or not (b).

of δ_{Nu} is below 10% for $Pe = 20$, $Pe = 10$, $Pe = 7$, $Pe = 5$, $Pe = 3$ and $Pe = 2$ at axial non-dimensional coordinate $\xi \geq 0.039$, $\xi \geq 0.081$, $\xi \geq 0.118$, $\xi \geq 0.17$, $\xi \geq 0.301$, $\xi \geq 0.478$, respectively. δ_{Nu} for $Pe = 100$ is always less than 7%, while δ_{Nu} for $Pe = 1$ is greater than 10% along the flow direction. This indicates that: (1) the axial conduction effect on asymptotic Nusselt number Nu_F can be neglected if $Pe > 10$. (2) its influence on local and asymptotic Nusselt number is negligible when $Pe > 100$. (3) if $Pe < 1$, the axial conduction must be considered.

The variation of Nu_L is examined at various values of Pe with $Kn = 0.04$ and $Br = -0.4$ to take the rarefied effect and viscous dissipation into consideration in Fig. 2.12b. When $\xi \geq 0.512$ (or $\xi \geq 0.375$), δ_{Nu} at $Pe = 10$ (or $Pe = 20$) is less than 10%. Also, δ_{Nu} at $Pe = 1$ is always high than 50% and δ_{Nu} at $Pe = 100$ is below 5%. Hence, similar conclusions about the axial conduction effect can be drawn when considering the rarefied effect and viscous dissipation. The consideration of Kn and Br effects induces a singular point at which Nu_L approaches infinity because the denominator θ_b vanishes (see Eq. (2.25)) at the critical point ξ_c as can be seen from Fig. 2.13b. Moreover, ξ_c gradually moves toward the inlet of the channel at larger Pe , which is in agreement with Fig. 2.9b.

Then the effects of axial conduction on the bulk non-dimensional temperature θ_b are examined, as shown in Fig. 2.13a. Here the rarefied effect and viscous dissipation are not considered by setting $Kn = 0$ and $Br = 0$. It is seen from the figure that, the rate of bulk temperature variation for $Pe = 1$ is obviously much slower than the other cases, as convection plays a more important role than conduction for extremely small Pe number. The relative difference of bulk temperature profile δ_θ ($\delta_\theta = \frac{\theta_b - \theta_b|_{Pe=10^6}}{\theta_b|_{Pe=10^6}}$) for $Pe = 100$ is less than 0.04 in all the fluid flow direction although $\theta_b|_{Pe=10^6}$ may cause other mathematical difference as this value tends to be 0 at the end of the channel. The effects of axial conduction on bulk dimensionless temperature, therefore, are negligible in the range $Pe > 100$. When the Kn effect and Br effect are accounted, as shown in Fig. 2.13b, similar results on the axial conduction can be observed.

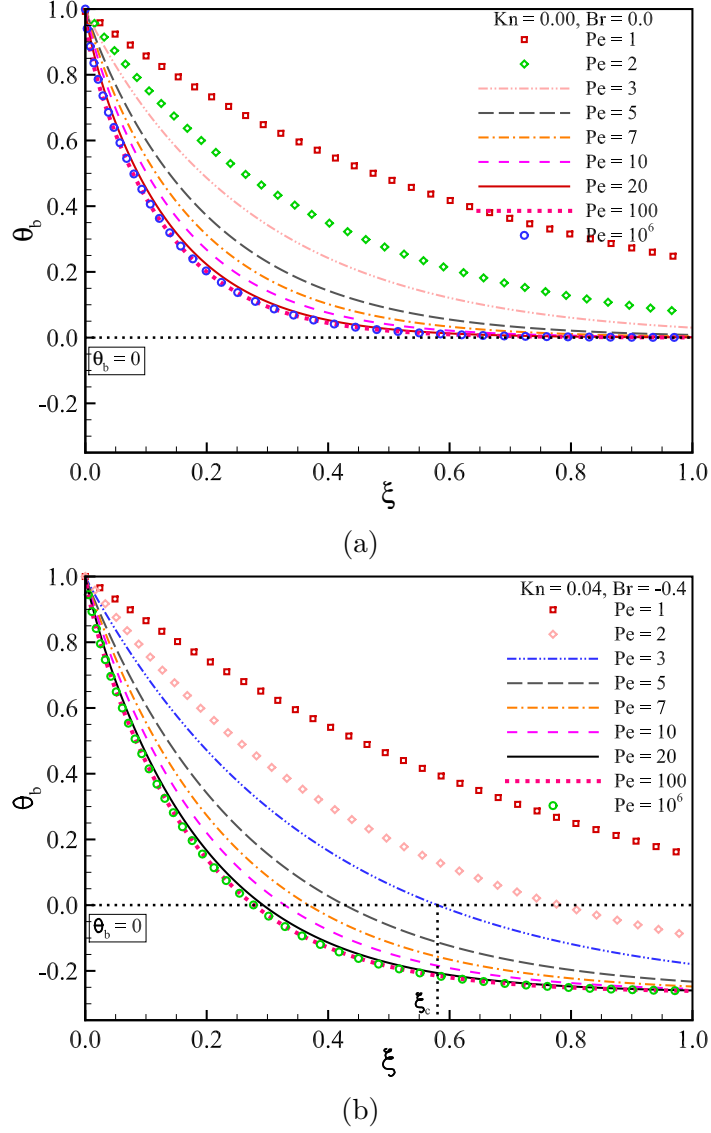


Figure 2.13: Bulk dimensionless temperature profile when neglecting rarefied effects and viscous dissipation (a) or not (b).

Rarefied effect

The effect of Kn number characterizing rarefaction on the local Nusselt number is examined, as described in Fig. 2.14. $Pe = 10^6$ and $Br = 0$ are adopted, leading to negligible axial conduction and viscous dissipation. Along the ξ axis, the Nusselt number only varies around the entrance and then reaches a constant value. The asymptotic Nusselt number Nu_F is 7.54 at $Kn = 0$ as reported in Section 2.1.6. Also, Nu_F decreases nonlinearly with the increasing of Kn .

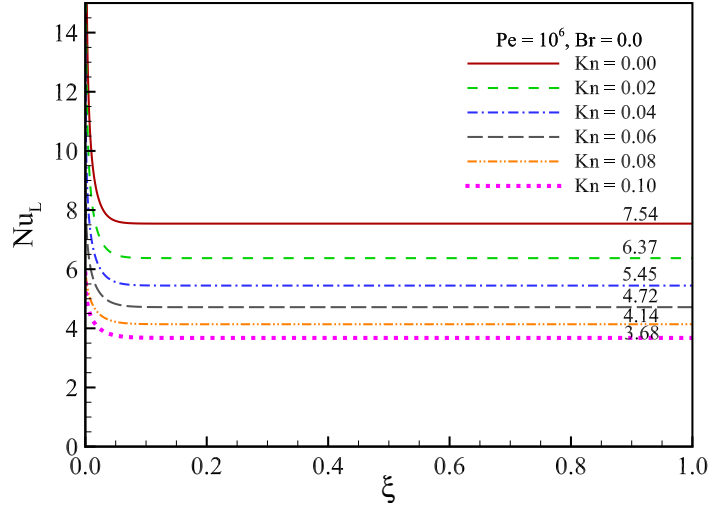


Figure 2.14: Rarefied effect on local Nusselt number.

As shown in Fig. 2.15, unlike the Nusselt number which approaches quickly to an asymptotic value in the axial direction, the fluid temperature jump occurs over the entire channel and becomes more obvious at higher Kn number. In addition, the temperature jump θ_s is 0 for $Pe = 10^6, Br = 0.00, Kn = 0.00$, and it can be also seen obviously that the fluid temperature near the wall is equal to zero from Eq. (2.5c) for the same case. This indicates that the truncation of the infinite series in Section 2.1.2 does not cause a significant difference in the analytical solution of the dimensionless energy equation and further validates the present method.

Fig. 2.16 is for the non-dimensional fluid bulk temperature distribution along the flow direction without axial conduction and viscous dissipation. Similarly with θ_s , the bulk temperature also varies across the whole channel. At $Kn = 0$, the bulk temperature keeps a constant value in the second half of the channel. This indicates that, in this continuous regime, heat transfer between the fluid and the solid materials only occurs around the first half of the channel. As Kn increases, however, the bulk temperature variation along the axis becomes more mild, revealing the potential to deliver cooling effect along the whole channel. This will be particularly useful when cooling

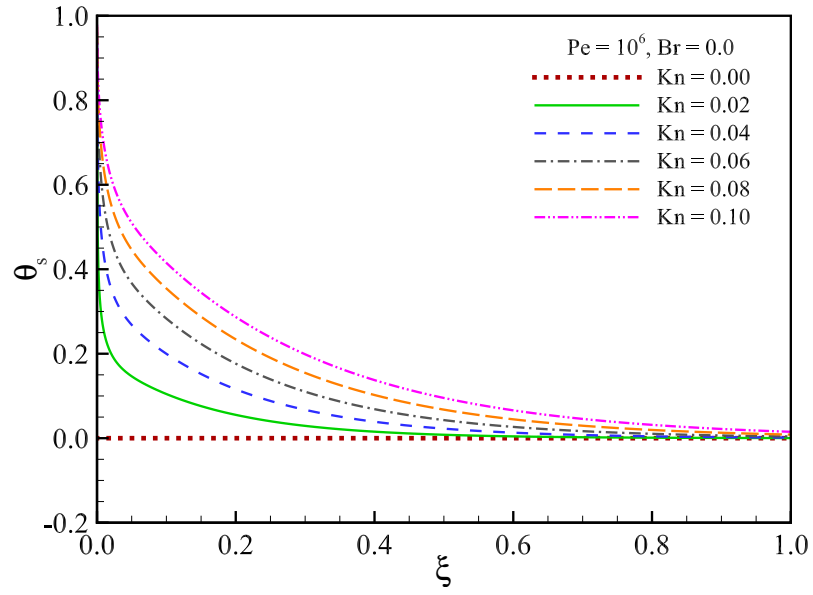


Figure 2.15: Rarefied effect on dimensionless temperature jump at the wall

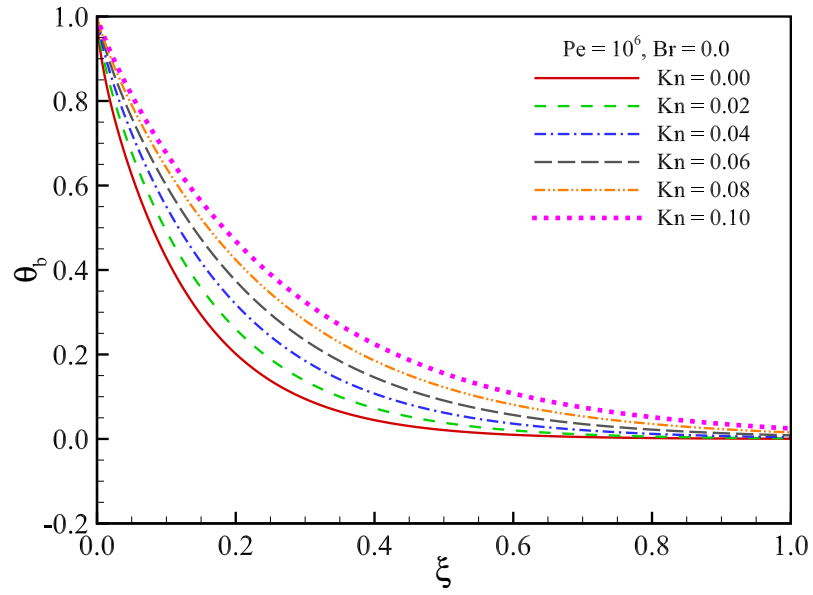


Figure 2.16: Rarefied effect on bulk dimensionless temperature.

a hot surface through micro or nanochannels.

2.2 Numerical simulation of resistance of velocity slip flow

2.2.1 The Navier velocity slip wall boundary condition

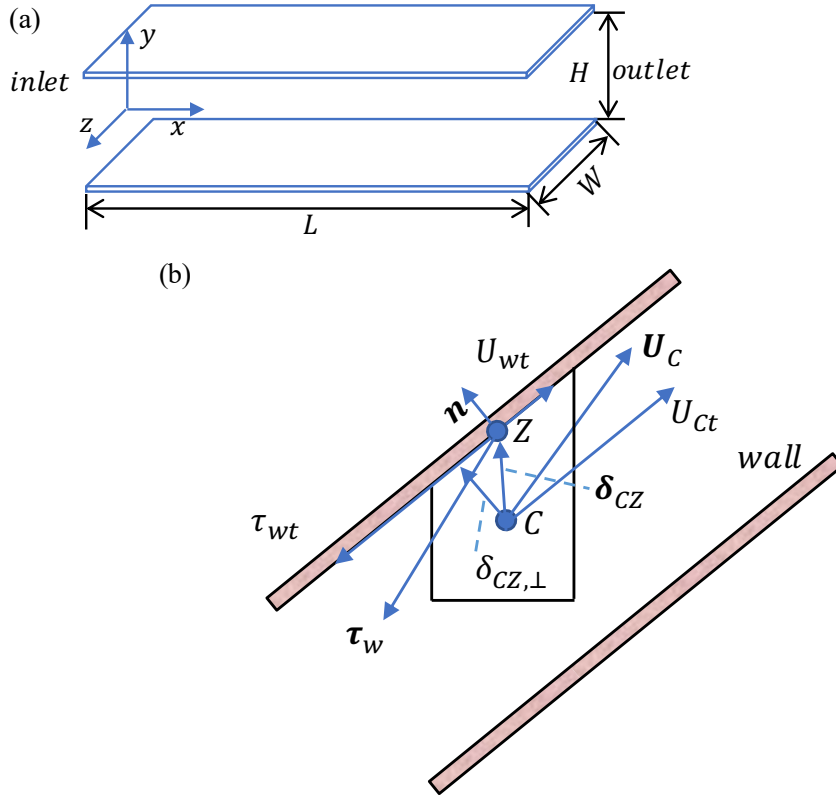


Figure 2.17: Sketches of (a) the plane parallel channel and (b) the near wall velocity slip.

The incompressible steady Newtonian flow through a plane parallel channel as shown in Fig. 3.1a is governed by the NS equations (Alokaily et al., 2019):

$$\nabla \bullet \mathbf{U} = 0 , \quad (2.48)$$

$$\nabla \bullet (\mathbf{U} \otimes \mathbf{U}) = -\nabla \frac{p}{\rho} + \nabla \bullet \left(\frac{\mu}{\rho} \nabla \mathbf{U} \right) , \quad (2.49)$$

where $\mathbf{U}$ is the velocity vector, $\mathbf{U} \otimes \mathbf{U} = \mathbf{U} \bullet \mathbf{U}^T$, p is the pressure, ρ is

the density and μ is the dynamic viscosity.

Considering that the mass flow rate is small enough to activate the partial boundary velocity slip, the normal component of $\mathbf{U}$ on the wall is zero (see Fig. 3.1b), and the tangential component on the wall, denoted as U_{wt} , is a function of the stress vector tangent to the wall τ_{wt} :

$$U_{wt} = \begin{cases} -S_l \tau_{wt}, & \text{linear} \\ -S_{nl} \tau_{wt} \|\tau_{wt}\|^{n-1}, & \text{nonlinear} \end{cases} \quad (2.50a)$$

$$(2.50b)$$

where $\|\tau_{wt}\|$ represents the l^2 norm of τ_{wt} , the negative signs indicate U_{wt} and τ_{wt} are in opposite directions, and S_l and S_{nl} are the linear and nonlinear slip coefficients, respectively (Navier, 1823; Fernandes et al., 2019). The present work will focus on the linear SBC, while the nonlinear counterpart commonly used for non-Newtonian fluids where the viscosity is dependent on shear rate (Feigl et al., 2016) can be implemented similarly.

For Newtonian flow, the fluid motion near the wall can be assumed as local Couette flow, therefore, the tangential wall stress vector τ_{wt} is

$$\tau_{wt} = \mu \frac{\partial U_t}{\partial \delta_{CZ,\perp}} = \mu \frac{U_{wt} - U_{Ct}}{\delta_{CZ} \bullet \mathbf{n}} = \mu \frac{(\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \bullet (\mathbf{U}_w - \mathbf{U}_C)}{\delta_{CZ} \bullet \mathbf{n}}, \quad (2.51)$$

where μ is the dynamic viscosity, C is the central point of the mesh cell next to the wall, Z is the central point of a boundary face, δ_{CZ} is the vector between this two points and $\delta_{CZ,\perp}$ is the projection of δ_{CZ} in the direction of $\mathbf{n}$. $\mathbf{U}_w$ and $\mathbf{U}_C$ are the velocity vector at Z and C , respectively and U_{wt} and U_{Ct} are their tangential components. $\mathbf{I}$ is the third-order unit matrix and $\mathbf{n}$ is the normal vector to the boundary face.

Substituting Eq. (2.51) into Eq. (2.50a), the linear SBC can be obtained

as

$$U_{wt} = -L_{slip} \frac{(\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \bullet (\mathbf{U}_w - \mathbf{U}_C)}{\delta_{CZ} \bullet \mathbf{n}}, \quad (2.52)$$

where L_{slip} ($L_{slip} = S_l \mu$) is the velocity slip length (Ng and Sun, 2017; Ng and Xie, 2018).

The tangential velocity of the fluid in the vicinity of the wall representing the Navier slip boundary conditions can be modelled via three schemes, denoted as explicit (Eq. (2.53a)), semi-implicit A (Eq. (2.53b)) and semi-implicit B (Eq. (2.53c)) (see Ferrás et al., 2013):

$$U_{wt}^i = \begin{cases} -L_{slip} \frac{(\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \bullet (\mathbf{U}_w^{i-1} - \mathbf{U}_C^{i-1})}{\delta_{CZ} \bullet \mathbf{n}}, & (2.53a) \end{cases}$$

$$U_{wt}^i = \begin{cases} -L_{slip} \frac{(\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \bullet (\mathbf{U}_w^i - \mathbf{U}_C^{i-1})}{\delta_{CZ} \bullet \mathbf{n}}, & (2.53b) \end{cases}$$

$$U_{wt}^i = \begin{cases} C_1 \mathbf{U}_C^i + (\mathbf{U}_w^{i-1} - C_1 \mathbf{U}_C^{i-1}), & (2.53c) \end{cases}$$

where the superscripts i and $i - 1$ denote values of corresponding quantities at the current or former time step, respectively. In the explicit scheme, relaxation is commonly implemented to improve the stability and convergence property when using large spatial or temporal intervals (Ferrás et al., 2013); in the semi-implicit A scheme, the bisection method is applied; in the semi-implicit B scheme, coefficient C_1 in Eq. (2.53c) is

$$C_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} - \left[(1 - C_2) \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} + C_2 \begin{pmatrix} n_x^2 \\ n_y^2 \\ n_z^2 \end{pmatrix} \right], \quad (2.54)$$

where $C_2 = L_{slip}/(\delta_{CZ} \bullet \mathbf{n} + L_{slip})$, and n_x , n_y and n_z are the three components of the normal vector $\mathbf{n}$. The details of this scheme are documented in Appendix B.

2.2.2 Resistance coefficient derived from the exact solution of the NS equations

The velocity profile for fully developed laminar flow through a plane parallel channel as shown in Fig. 1a with linear SBC can be obtained from Eq. (2.48) and Eq. (2.49):

$$U_x = -\frac{1}{2\mu} \frac{dp}{dx} \left(\frac{H^2}{4} + L_{slip}H - y^2 \right), \quad (2.55)$$

where H is the height of the channel, and this velocity profile is in agreement with references (Sun et al., 2020). Then the average velocity can be calculated from

$$U_m = \frac{\int_{-\frac{H}{2}}^{\frac{H}{2}} U_x dy}{H} = -\frac{1}{12\mu} \frac{dp}{dx} (H^2 + 6L_{slip}H). \quad (2.56)$$

In general, the pressure loss over a streamwise length L for all types (laminar or turbulent, circular or noncircular, smooth or rough surfaces, horizontal or inclined pipes) of fully developed internal flows can be represented as (Sheikholeslami and Ganji, 2016)

$$\Delta p = K \frac{\rho U_m^2}{2}, \quad (2.57)$$

where K is named the flow resistance coefficient, which measures the efficiency of the mass transfer.

Considering that the pressure gradient is constant, or $\Delta p/L = dp/dx$ and combining Eq. (2.56) and Eq. (2.57), K for fully developed laminar flow in

a plane parallel channel with linear SBC can be obtained as

$$K = \frac{24}{Re \left(1 + 6 \frac{L_{slip}}{H}\right)} \frac{L}{H}, \quad (2.58)$$

where Re is the Reynolds number based on the average velocity and the channel height H .

Similarly the flow resistance coefficient in a fully developed laminar pipe flow with SBC can be obtained:

$$K = \frac{64}{Re \left(1 + 8 \frac{L_{slip}}{D}\right)} \frac{L}{D}. \quad (2.59)$$

The first factor on the right of Eq. (2.58) and Eq. (2.59) represents the friction factor. Clearly in Eq. (2.59) when the no-slip condition is imposed ($L_{slip} = 0$), there is $K = 64/Re$, a well known formula for the macro-scale laminar pipe flow. Moreover, the wall friction coefficient (f) can be defined as the ratio of the shear stress and fluid velocity at the wall, and subsequently there is $f = \mu/L_{slip}$ from Eq. (2.51) and Eq. (2.55). This indicates the wall friction coefficient is inversely proportional to the velocity slip length at constant fluid viscosity, in agreement with the experimental work (Wu et al., 2014).

2.2.3 Resistance coefficient calculated from SLA

As an alternative to the definition, it has been proposed that K can be obtained from SLA for non-slip flow (Herwig and Schmandt, 2014):

$$K = \frac{T \dot{S}_{irr,D}}{\rho \frac{U_m^3}{2} A}, \quad (2.60)$$

where T is the temperature, $\dot{S}_{irr,D}$ is the generation rate of entropy due to thermodynamic irreversibility, and $T\dot{S}_{irr,D}$ corresponds to the rate of the exergy loss according to the Gouy–Stodola theorem (Baehr and Kabelac, 2009).

When the SLA method is used to calculate K for the slip flow from the view of the balance of energy, the skin friction drag does negative work on the fluid (which is zero at the no-slip condition). In other words, the head loss of fluid is caused by two factors: viscous dissipation and skin friction drag. Therefore, the definition of the resistance coefficient should be adjusted to take into account this term as

$$K = \frac{T\dot{S}_{irr,D} + W_{drag}}{\rho \frac{U_m^3}{2} A}, \quad (2.61)$$

where W_{drag} represents the contribution of the wall skin friction on fluid, and it can be calculated from Eq. (2.51) and Eq. (2.55) as

$$W_{drag} = \left| \int_S \tau_{wt} \bullet U_{wt} dS \right| = \frac{72\mu U_m^2 L W H^2 L_{slip}}{(H^2 + 6L_{slip}H)^2}. \quad (2.62)$$

Bejan (Bejan, 1982) proposed that the volumetric rate of entropy generation consists of the volumetric rate of the heat transfer irreversibility and the fluid friction irreversibility. For steady, isothermal and incompressible channel flow without or with linear SBC considered in the present work, the local entropy generation rate is only from the fluid friction irreversibility and can be computed from

$$\dot{S}_{irr,D}''' = \frac{1}{T} \boldsymbol{\tau} : \boldsymbol{\nabla} \mathbf{U} = 144 \frac{\mu}{T} \frac{y^2}{(H^2 + 6L_{slip}H)^2} U_m^2. \quad (2.63)$$

The overall entropy production rate can be obtained by integrating the local entropy generation rate:

$$\dot{S}_{irr,D} = \int_V \dot{S}_{irr,D}''' dV = \frac{12\mu WL}{T} \frac{H^3 U_m^2}{(H^2 + 6L_{slip}H)^2}. \quad (2.64)$$

Substituting Eq. (2.62) and Eq. (2.64) and into Eq. (2.61), the flow resistance coefficient is

$$K = \frac{24}{Re} \frac{1}{1 + 6\frac{L_{slip}}{H}} \frac{L}{H}, \quad (2.65)$$

the same as Eq. (2.58) derived from the NS equations. Similarly the resistance coefficient in a fully developed laminar pipe flow with SBC can be obtained and it also matches that from the NS method (see Eq. (2.59)).

2.2.4 Validation

Table 2.3: Resistance coefficient for plane channel and circular pipe flow

	method	NS	SLA
channel	theoretical	0.2427	0.2427
	explicit scheme	0.2403	0.2431
	semi-implicit scheme A	0.2415	0.2429
	semi-implicit scheme B	0.2415	0.2452
pipe	theoretical	0.6009	0.6009
	explicit scheme	0.5986	0.6024
	semi-implicit scheme A	0.6008	0.6034
	semi-implicit scheme B	0.6014	0.6094

Numerical simulations are performed to validate the derivations in Section 2.2.3. The plane parallel channel shown in Fig. 3.1a with $L = 30\text{ mm}$, $W = 0.2\text{ mm}$ and $H = 2\text{ mm}$ is adopted. A circular pipe with length and diameter $L = 30\text{ mm}$ and $D = 2\text{ mm}$, respectively, is also considered. The density of water is $\rho = 997.05\text{ kg/m}^3$, and its dynamic viscosity is $\mu = 8.90 \times 10^{-4}\text{ Pa} \cdot \text{s}$. The average velocity for no-slip or slip flow is

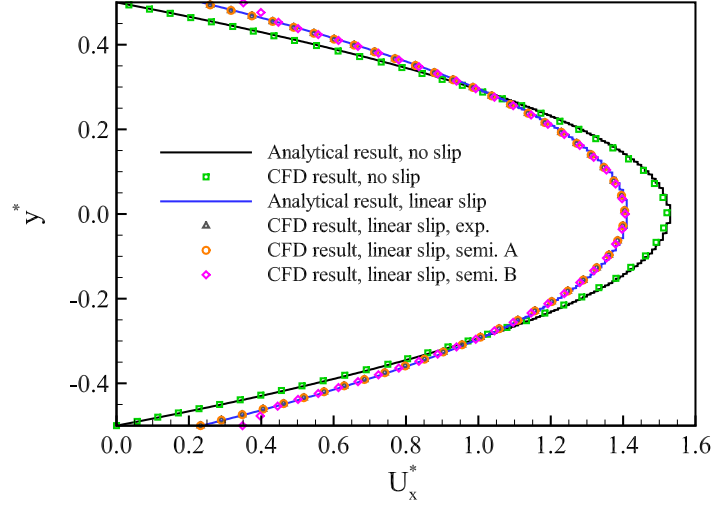


Figure 2.18: Velocity profile in a channel flow, where $y^* = y/H$ and $U_x^* = U_x/U_m$.

$U_m = 0.50929 \text{ m/s}$ and the slip length is $L_{slip} = 10^{-4} \text{ m}$. $\Delta t = 10^{-4} \text{ s}$ was chosen as the time step to ensure that the maximum Courant number is less than 1. The coupling of pressure and velocity is addressed by the PISO algorithm.

The streamwise velocity and coordinate system are non-dimensionalised by average velocity U_m and channel height H , respectively. Fig. 2.18 shows the dimensionless streamwise velocity profiles along the height direction of the plane channel (velocity distributions in a circular pipe are not shown here for conciseness). The simulation results are in excellent agreement with the analytical outcomes. Furthermore, the explicit scheme leads to well agreed velocity distributions. The resistance coefficients for fully developed slip flow in the plane parallel channel and the circular pipe calculated from the NS equations and the SLA approach are in good agreement with each other, as shown in Table 2.3. This validates the analytical derivations presented in Section 2.2.3 and demonstrate the accuracy of the aforementioned explicit scheme of the linear SBC.

2.2.5 Flow resistance in a channel with an SCC

Problem descriptions

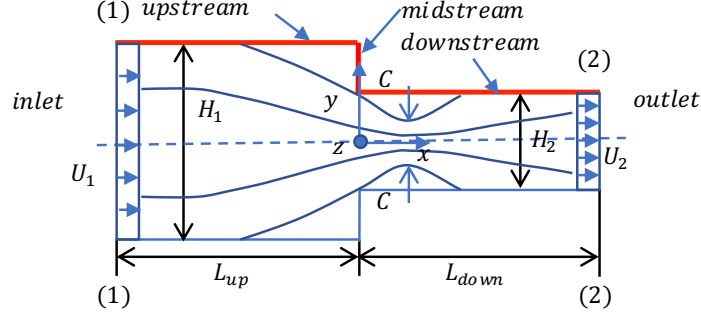


Figure 2.19: Schematic of flow through an SCC.

After investigating the efficiency of mass transfer in a straight channel, the flow resistance coefficient through an SCC as schematically illustrated in Fig. 2.19 will be examined using both the NS and the SLA approaches. The total flow resistance consists of the loss in the upstream large channel, downstream small channel and the SCC.

By definition, the flow resistance coefficient K_{SCC} induced by the SCC can be written as

$$K_{SCC} = \frac{1}{\rho \frac{U_2^2}{2}} \left[\Delta p - \Delta p_{up,\circ} - \Delta p_{down,\circ} + \frac{\rho (U_1^2 - U_2^2)}{2} \right], \quad (2.66)$$

where $\Delta p_{up,\circ}$ and $\Delta p_{down,\circ}$ denote the pressure loss of fully developed laminar flow in the upstream and downstream channel without SCC, respectively, and they can be determined from Eq. (2.57) and Eq. (2.58). U_2 is the average velocity at the outlet and will be used as the characteristic velocity, and Δp is the pressure difference between inlet and outlet.

K_{SCC} can also be obtained from the SLA method through re-writing Eq. (2.61)

$$\begin{aligned} K_{SCC} &= \frac{1}{\rho \frac{U_2^3}{2} A} \left(T \dot{S}_{irr, D, SCC} + W_{D, SCC} \right) \\ &= \frac{1}{\rho \frac{U_2^3}{2} A} \left[(T \dot{S}_{irr, D, total} + W_{D, total}) - (T \dot{S}_{irr, D, up, \circ} + \right. \\ &\quad \left. W_{D, up, \circ}) - (T \dot{S}_{irr, D, down, \circ} + W_{D, down, \circ}) \right] . \end{aligned} \quad (2.67)$$

where $T \dot{S}_{irr, D, up, \circ}$ and $T \dot{S}_{irr, D, down, \circ}$ represent the entropy production rate of flow that is not affected by the SCC in the upstream and downstream channel, respectively. These terms are calculated from Eq. (2.64) when considering no-slip or linear SBC. $W_{D, up, \circ}$ and $W_{D, down, \circ}$ are the work contributed by wall skin friction, and can be obtained from Eq. (2.62). A is the area of the cross section of the downstream channel. Also, the overall flow resistance coefficient K_{total} of this SCC could be determined directly from Eq. (2.61).

The height of the downstream channel H_2 is set to $2 \times 10^{-5} m$ and used as the characteristic length, resulting in $L_{slip}^* = L_{slip}/H_2$. H_1/H_2 represents the contraction ratio and will be denoted as R_{area} . The upstream and downstream lengths of the channel are $L_{up}/H_2 = 25$ and $L_{down}/H_2 = 50$, respectively, which have been found to be long enough to accommodate the flow affected by the SCC. Moreover, the wall shear stress and the drag force work will be non-dimensionalised by ρU_2^2 and $\rho U_2^3 H_2^2$, respectively. The time step for each case is adjusted to ensure that the maximum Courant number is less than 1.

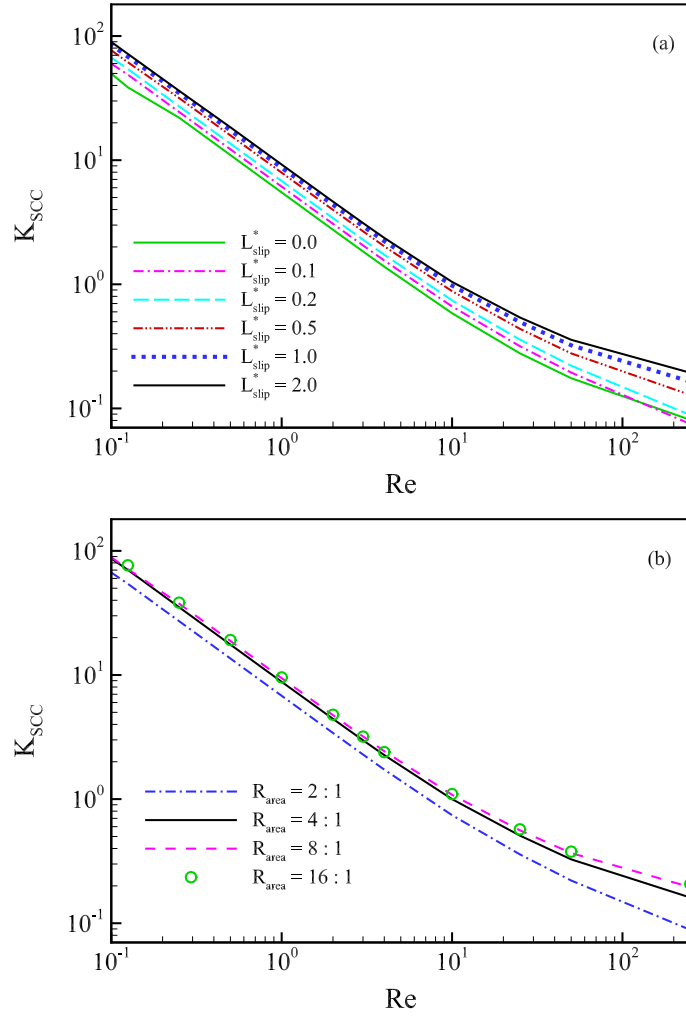


Figure 2.20: Flow resistance coefficient of the SCC calculated from the SLA method at various Re and L_{slip}^* . (a) $R_{area} = 2 : 1$, (b) $L_{slip}^* = 0.2$.

The flow resistance coefficient

The flow resistance coefficient K_{SCC} of the SCC computed from Eq. (2.66) and Eq. (2.67) is shown in Fig. 2.20. Unlike the resistance coefficient in the macro turbulent flow which is only dependent on the cross section ratio and insensitive to Re , K_{SCC} in the present micro channel drops rapidly with increasing Re . Fig. 4b shows the effect of the contraction ratio R_{area} on the flow resistance coefficient K_{SCC} . At prescribed Re and L_{slip}^* , one can find that K_{SCC} increases slightly with the contraction ratio R_{area} . Through data fitting, the resistance coefficient over low Re (e.g., $Re \leq 10$) can be

modelled as

$$K_{SCC} \approx \frac{aL_{slip}^{*3} + bL_{slip}^{*2} + cL_{slip}^{*} + d}{Re}, \quad (2.68)$$

where coefficients (a, b, c, d) are constants at prescribed R_{area} , and are $(1.401, -5.518, 7.299, 5.488)$ and $(0.2283, -1.338, 2.747, 8.35)$ for $R_{area} = 2 : 1$ and $4 : 1$, respectively. At $R_{area} \geq 8 : 1$, (a, b, c, d) converges to $(0.4454, -1.894, 2.917, 8.909)$, offering a formula for quick estimation of the resistance coefficient at small Reynolds numbers and large contraction ratios with a given velocity slip length. One should note that the fitting equation underestimates the resistance coefficient at larger Re .

In addition, K_{SCC} can be transformed to the equivalent length of undisturbed fully developed downstream flow with the same flow resistance

$$L_{equi}^{*} = \frac{L_{equi}}{H_2} = \frac{1}{24} Re K_{SCC} (1 + 6L_{slip}^{*}) . \quad (2.69)$$

The dimensionless equivalent length L_{equi}^{*} increases with respect to L_{slip}^{*} , but is insensitive to Re when Re is small enough as shown in Fig. 2.21, where R_{area} is fixed at 4:1 and the numerically computed K_{SCC} is adopted. This can be also demonstrated analytically by substituting Eq. (2.68) into Eq. (2.69), which results in a Re -independent L_{equi}^{*} . However at higher Re (e.g. $Re \geq 10$), the analytical fitting equation underestimates the resistance coefficient K_{SCC} and consequently L_{equi}^{*} , as confirmed by the numerical results in Fig. 2.21. Variations of L_{equi}^{*} at other R_{area} are similar and are not shown here.

Above we reported effects of Re , L_{slip}^{*} and R_{area} on the flow resistance coefficient K_{SCC} and dimensionless equivalent length L_{equi}^{*} . In the following sections, the fluid physics will be explored and efforts will be focused on the two sources of the flow resistance, i.e., drag force work and viscous dissipation loss.

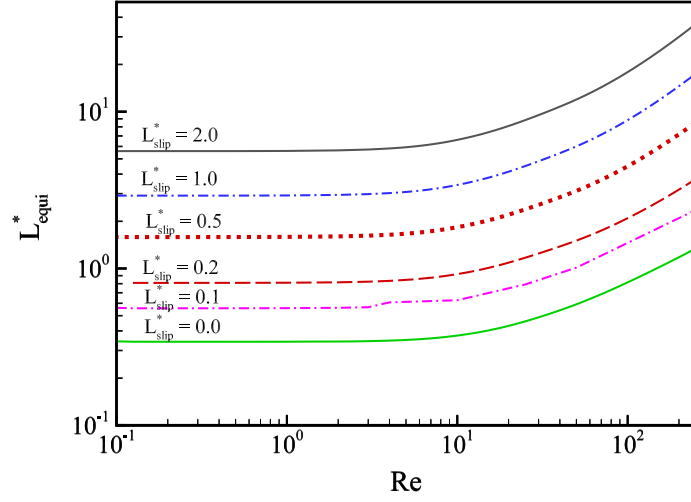


Figure 2.21: The equivalent length of the resistance coefficients at various Re and L_{slip}^* at $R_{area} = 4 : 1$.

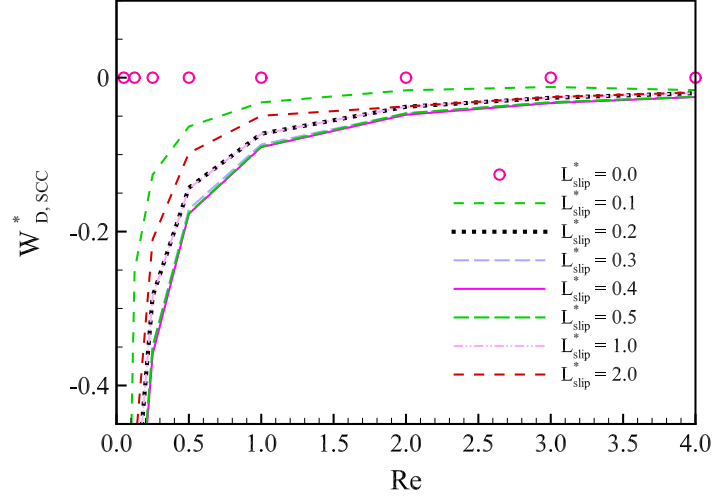


Figure 2.22: Wall shear tangential stress work of the SCC at various Re and L_{slip}^* at $R_{area} = 4 : 1$.

Wall shear stress vector and drag force work

The dimensionless drag force work of the SCC, $W_{D,SCC}^*$, increases with Re number for velocity slip flow as shown in Fig. 2.22. Furthermore, there is a critical dimensionless velocity slip length ($L_{slip,cri}^* \approx 0.4$ for all the four R_{area} studied) where $W_{D,SCC}^*$ reaches its minimum. One should note that $W_{D,SCC}^*$ is almost always less than 0 (the reason will be illustrated later), indicating that the drag force work tends to reduce the flow resistance coefficient of the SCC according to the definition in Eq. (2.67).

2.2. NUMERICAL SIMULATION OF RESISTANCE OF VELOCITY SLIP FLOW

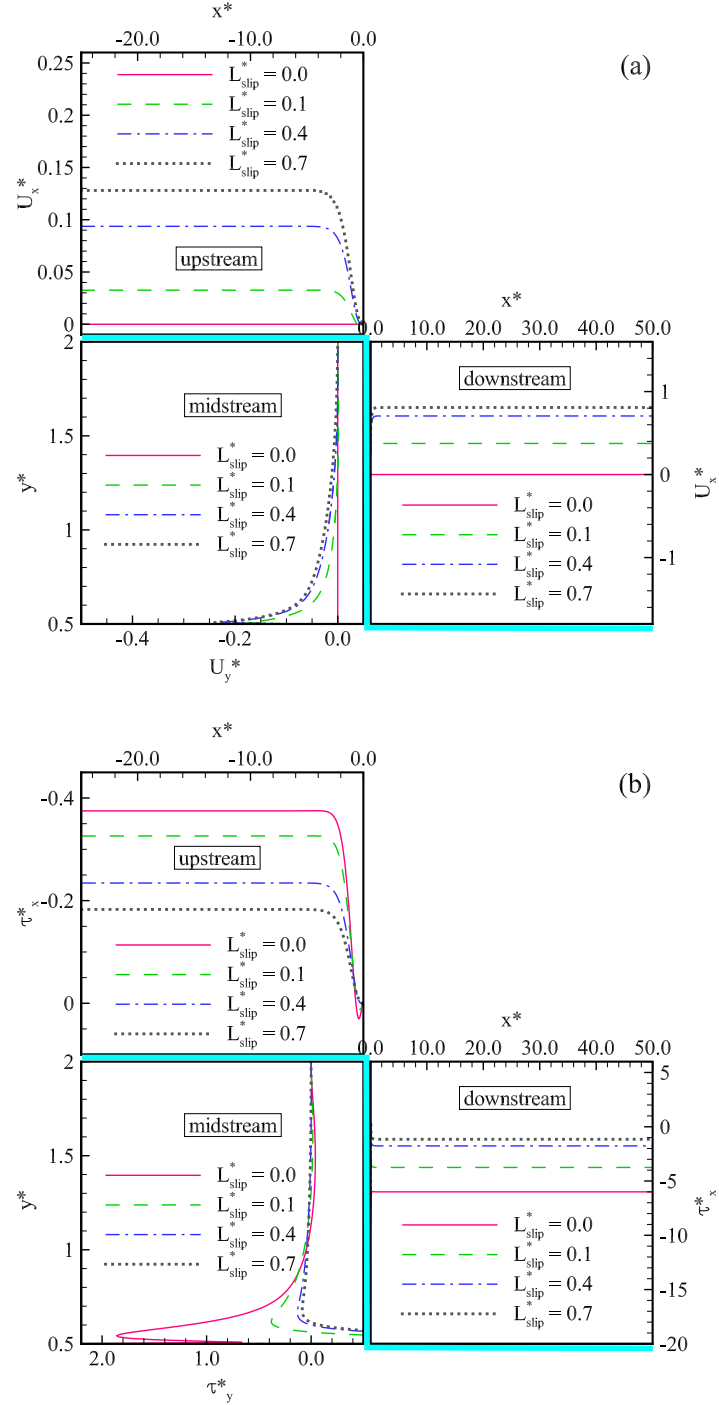


Figure 2.23: Streamwise (upstream and downstream sections) and vertical (midstream section) velocity on the wall (a) and shear stress (b) profiles at various L_{slip}^* at $R_{area} = 4 : 1$, $Re = 1$ (the shallow green edges represent upstream, midstream and downstream channel as illustrated in Fig. 2.19).

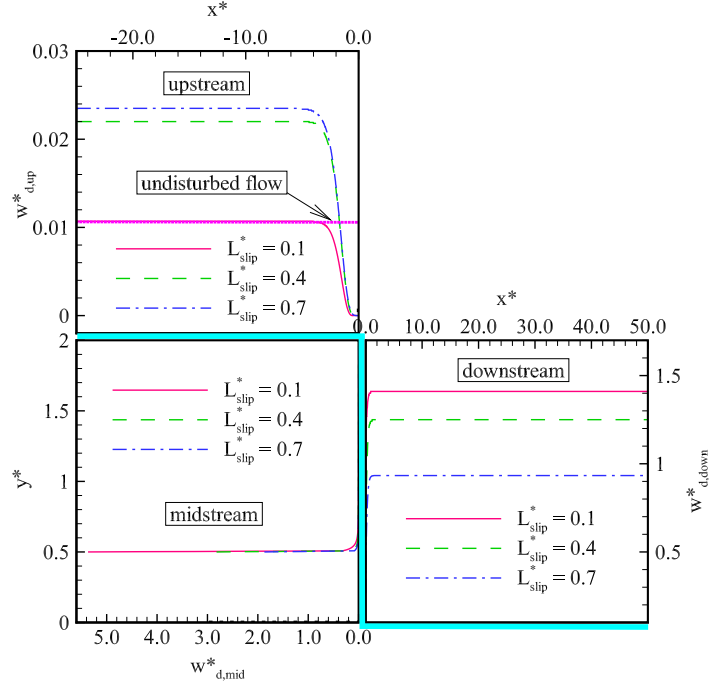


Figure 2.24: Drag work per unit area at various L_{slip}^* when $R_{area} = 4 : 1$ and $Re = 1$ (the shallow green edges represent upstream, midstream and downstream channel as illustrated in Fig. 2.19).

Fig. 2.23 describes how L_{slip}^* affects the dimensionless wall velocity and shear stress distributions for the upstream, midstream and downstream of the SCC shown in Fig. 2.19 at $R_{area} = 4 : 1$ (results for other contraction ratios are similar and are not shown here for brevity). Away from the SCC, the dimensionless velocity and wall shear stress maintain constant values that match the velocity and shear stress in the straight channel flow from analytical calculations. The magnitude of near wall velocity enlarges with increasing L_{slip}^* . Conversely, the amplitude of the upstream and downstream wall shear stress τ_x^* for slip flow are far less than $|\tau_x^*|$ for no-slip flow at a prescribed Re , and this is in agreement with the experimental observation (Wu et al., 2014).

The dimensionless drag force work per unit area w_d^* for the SCC with $R_{area} = 4 : 1$ is plotted in Fig. 2.24 to explain the negative value of $W_{D,SCC}^*$ mentioned above. In terms of the dimensionless tangential wall shear stress

work of the SCC in Fig. 2.22, $W_{D,SCC}^*$ can be rewritten as

$$W_{D,SCC}^* = (W_{D,up}^* - W_{D,up,\circ}^*) + W_{D,mid}^* + (W_{D,down}^* - W_{D,down,\circ}^*) . \quad (2.70)$$

The region of the downstream channel affected by the SCC is very small according to Fig. 2.24 and $w_{d,down}^*$ is almost constant rendering the third term of the right side of Eq. (2.70) close to 0. Furthermore, $W_{D,mid}^*$ is essentially very small resulting in $W_{D,SCC}^* \approx W_{D,up}^* - W_{D,up,\circ}^*$. From Fig. 2.24, one can observe that $w_{d,up}^*$ affected by the SCC is equal to $w_{d,up,\circ}^*$ at most part of the upstream channel, and becomes smaller than $w_{d,up,\circ}^*$ at the end of the upstream channel. This leads to a negative value of $W_{D,SCC}^*$, as observed before in Fig. 2.22.

Disturbed region and local entropy generation rate

To examine the range of regions affected by the SCC, a non-dimensional surface integral of the local entropy production rate is defined as

$$\dot{S}_{irr,D}^{\prime,*} = \frac{\dot{S}_{irr,D}^{\prime}}{\dot{S}_{irr,D,\circ}^{\prime}} = \frac{\int_A \dot{S}_{irr,D}^{\prime\prime\prime} dA}{\int_A \dot{S}_{irr,D,\circ}^{\prime\prime\prime} dA} , \quad (2.71)$$

where A is an arbitrary cross section area. $\dot{S}_{irr,D,\circ}^{\prime\prime\prime}$ represents the local entropy production rate of flow without SCC and its surface integral can be formulated based on Eq. (2.64).

The non-dimensional length of upstream and downstream channel domain affected by the SCC can be defined as

$$L_{up,dist}^* = \frac{|0 - x_{up,dist}|}{H_2}, L_{down,dist}^* = \frac{|x_{down,dist} - 0|}{H_2} , \quad (2.72)$$

where $x_{up,dist}$ and $x_{down,dist}$ are x coordinates of the disturbed points where

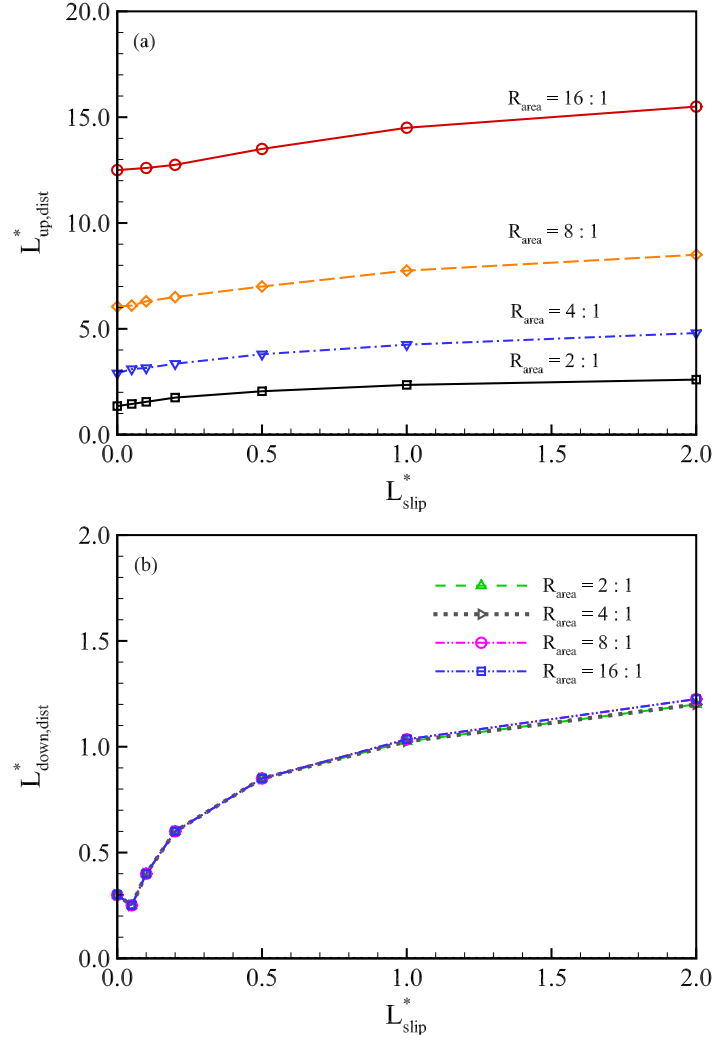


Figure 2.25: Dimensionless length of the disturbed domain at $Re = 0.5$. (a) upstream, (b) downstream.

$\dot{S}'_{irr,D}|_{x=x_{up,dist}} = 0.95$ and $\dot{S}'_{irr,D}|_{x=x_{down,dist}} = 0.95$, respectively (Herwig and Schmandt, 2014). 0 represents the x coordinate of the position of the SCC, where the area of the cross section changes abruptly. As shown in Fig. 2.25, $L_{up,dist}^*$ and $L_{down,dist}^*$ are almost independent on Re and increase with L_{slip}^* . In addition, $L_{up,dist}^*$ rises conspicuously and $L_{down,dist}^*$ remains almost constant with increasing R_{area} .

Contours of $T\dot{S}'''_{irr,D}$ are shown in Fig. 2.26 from which we can observe the viscous dissipation loss of fluid at every point in the flow field and the effects of Re , L_{slip}^* and R_{area} . Comparing Fig. 2.26a with Fig. 2.26b, the viscous

2.2. NUMERICAL SIMULATION OF RESISTANCE OF VELOCITY SLIP FLOW

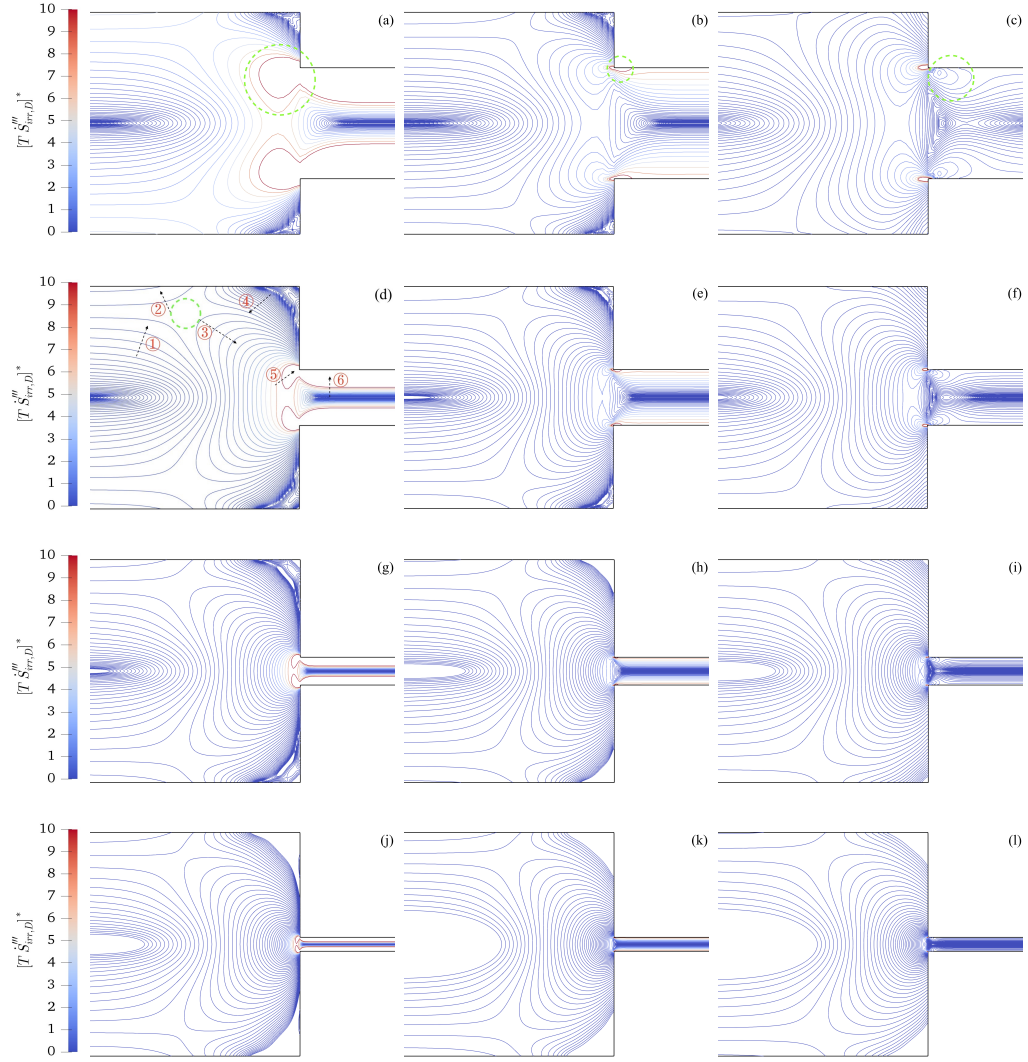


Figure 2.26: Contours of local entropy generation rate $\dot{S}'''_{irr,D}$ at per unit temperature non-dimensionalised by $\rho U_2^3/H_2$ at various Re , L^*_{slip} and R_{area} . (a) $Re = 0.5$, $L^*_{slip} = 0.0$, $R_{area} = 2 : 1$, (b) $Re = 4.0$, $L^*_{slip} = 0.0$, $R_{area} = 2 : 1$, (c) $Re = 4.0$, $L^*_{slip} = 0.5$, $R_{area} = 2 : 1$, (d) $Re = 0.5$, $L^*_{slip} = 0.0$, $R_{area} = 4 : 1$, (e) $Re = 4.0$, $L^*_{slip} = 0.0$, $R_{area} = 4 : 1$, (f) $Re = 4.0$, $L^*_{slip} = 0.5$, $R_{area} = 4 : 1$, (g) $Re = 0.5$, $L^*_{slip} = 0.0$, $R_{area} = 8 : 1$, (h) $Re = 4.0$, $L^*_{slip} = 0.0$, $R_{area} = 8 : 1$, (i) $Re = 4.0$, $L^*_{slip} = 0.5$, $R_{area} = 8 : 1$, (j) $Re = 0.5$, $L^*_{slip} = 0.0$, $R_{area} = 16 : 1$, (k) $Re = 4.0$, $L^*_{slip} = 0.0$, $R_{area} = 16 : 1$, (l) $Re = 4.0$, $L^*_{slip} = 0.5$, $R_{area} = 16 : 1$.

dissipation loss further concentrates on the corner as marked by the green circles in these two subfigures at larger Re . One interesting observation is that an "ear" type dissipation loss region appears at the beginning section of the downstream channel for slip flow, as marked by the green circle in Fig. 2.26c.

Moreover, the local entropy production rate of fluid in the SCC consists of six sections, mainly including upstream and downstream channels and 90° corners, etc (see Fig. 2.26d). Conspicuously, $T\dot{S}_{irr,D}'''$ for flow of the upstream and downstream channel affected by the SCC increases from the center line of the SCC and peaks at the wall (see the arrow ① and ⑥ in Fig. 2.26d), suggesting that the viscous dissipation loss minimizes at the center line and enlarges along the height direction of upstream and downstream channels. $T\dot{S}_{irr,D}'''$ for the 90° corner ④ increases along the direction departing from the corner, and the variation trend is opposite to the other 90° corner ⑤ where the local entropy generation rate or flow resistance is the maximum in the whole flow field. The growth gradient for $T\dot{S}_{irr,D}'''$ at these two corners rises dramatically at larger Re . An interesting point is that there is a "source" (surrounded by the green circle in Fig. 2.26d) of $T\dot{S}_{irr,D}'''$, from which the flow resistance increases along with opposite directions (② and ③ in Fig. 2.26d).

2.3 Conclusions

In this chapter, First we obtain an infinite series solution of the 2D energy equation with a first-order velocity slip model and a first-order temperature jump model by applying the separation of variables method and the variable substitution approach, and the analytical solution is applied to study effects of the viscous dissipation, axial conduction and rarefaction on heat transfer. The following results can be drawn:

1. The asymptotic non-dimensional bulk temperature of fluid $|\theta_{bF}|$ converges to a constant value higher than the wall temperature regardless of the inlet condition at a given set of Pe , Br ($Br \neq 0$) and Kn . This

value increases linearly with Br , drops slightly at higher Kn , and is almost independent on Pe .

2. If a fluid is used to cool the wall with uniform temperature, there is a critical point where the fluid bulk temperature reaches the same value as wall temperature and the Nusselt number becomes ill-defined at this point. This point moves much closer to the channel entrance at increasing $|Br|$ or Pe . On the contrary, the point moves towards the end of the channel with increasing Kn .
3. By eliminating the rarefied effect and axial conduction, the asymptotic Nusselt number with or without viscous dissipation is 17.5 or 7.54, respectively.
4. The axial conduction effect on asymptotic Nusselt number can be neglected if $Pe > 10$ while the effect of axial conduction on the local Nusselt number and bulk non-dimensional temperature are negligible when $Pe > 100$.
5. The rarefied effect on the local Nusselt number is localized around the entrance of the channel, but is across the whole channel for the bulk temperature and temperature jump. At a larger Kn , the bulk temperature variation along the axis becomes milder, revealing the potential to deliver cooling effect along the whole channel.

Besides, the flow resistance coefficient in flow passing through a pipe or channel with or without a sudden contraction component (SCC) at low Reynolds number conditions with a slip wall velocity boundary condition implemented using the three schemes is analyzed using NS equations and the second law analysis (SLA) approach which is extended to determine and visualize the flow resistance loss of velocity slip flow after considering

the work contributed by wall drag force. Effects of Re and dimensionless velocity slip length (L_{slip}^*) on the flow resistance coefficient of laminar flow through the SCC with various contraction ratios (R_{area}) are revealed.

At $Re \leq 10$, the flow resistance coefficient for the SCC, denoted as K_{SCC} , increases monotonously with L_{slip}^* and $1/Re$ and nonlinearly with R_{area} , and at $R_{area} \geq 8$, the resistance coefficient can be modelled as $K_{SCC} = (0.4454L_{slip}^{*3} - 1.894L_{slip}^{*2} + 2.917L_{slip}^* + 8.909)/Re$.

Physically, the flow resistance of fluids results from two factors: wall drag force work (equal to 0 for no-slip flow) and viscous dissipation in the flow field related to the local entropy generation rate. These two terms are computed and analyzed individually to illustrate the fluid physics underpinning the flow resistance.

The amplitude of the negative drag work ($W_{D,SCC}^*$) decreases monotonously at larger Re . Also, there is a critical velocity slip length at which the amplitude of $W_{D,SCC}^*$ reaches maximum. In terms of fluid internal viscous dissipation, it minimizes at the center line and peaks at the wall of the upstream and the downstream channel. Moreover, the dissipation loss concentrates around the end section of the upstream channel of the SCC.

Both the dimensionless lengths of the disturbed region of the upstream and downstream channels are almost independent on Re and enlarge at larger L_{slip}^* . With increasing R_{area} , the former rises remarkably while the latter remains nearly a constant value.

Chapter 3

Molecular dynamics simulation of liquid argon flow in a nanoscale channel

In Chapter 2, the effects of the slip phenomenon on the heat transfer and flow resistance are clarified based on the continuum-based governing equations. However, the applied slip models include constant momentum and thermal accommodation coefficients that strongly depend on many factors such as materials of fluids and the wall, local pressure, velocity and the mean direction of the local flow, etc. Also, the continuum-based governing equations become less valid when depicting nanoscale flow and heat transfer problems due to the violation of the non-uniform density and viscosity profiles, as reported in Section 1.4. In this chapter, therefore, fluid and heat transfer in a nanoscale channel is investigated by molecular dynamics simulations. Results are then compared with those from the continuum-based governing equations to (1) evaluate the validity of the continuity assumption, (2) determine the influence factors of velocity and temperature slips,

and (3) reveal the physical characteristics of Micro/Nanoscale flow and heat transfer such as non-uniform density and viscosity profiles. Technical details pertaining to MD simulations are illustrated in Section 3.1, and the results and discussions are presented in Section 3.2 and Section 3.3. Finally, conclusions are drawn in Section 3.4.

3.1 Methodology of molecular dynamics simulations

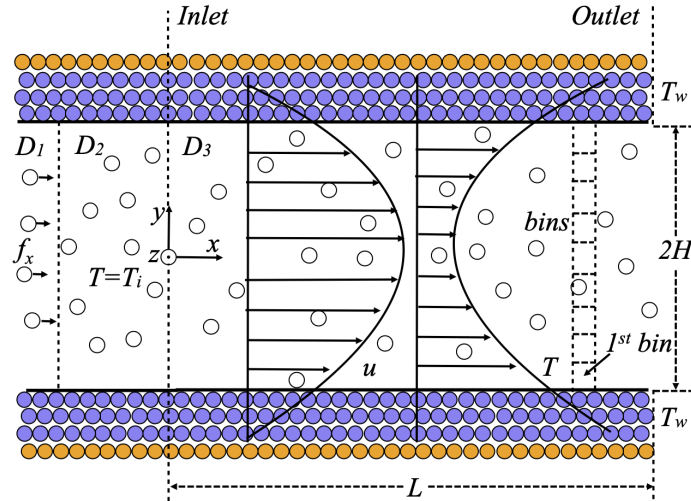


Figure 3.1: Sketch of the MD simulation system. The modelling domain includes three sub-domains: forcing region D_1 , thermostat region D_2 and sample region D_3 . Open circles denote liquid argon atoms. The outermost wall atoms (brown circles) are frozen to their initial positions, and the other wall atoms (blue circles) are constrained to corresponding initial locations via virtual springs.

3.1.1 Governing equations

As shown in Fig. 3.1, the liquid argon atoms are delivered along the x direction in a parallel plate channel composed of solid silver atoms with the face-centered structure (FCC) and lattice constant $4 \text{ \AA}$. Periodic boundary

conditions are applied in x and z directions. The motions of particles are governed by

$$\mathbf{f}_{ij} = -\nabla U(r_{ij}), \quad (3.1a)$$

$$m\ddot{\mathbf{r}}_i = \mathbf{f}_i = \sum_{j=1, j \neq i}^{N_m} \mathbf{f}_{ij}, \quad (3.1b)$$

where $U(r_{ij})$ is the potential energy function, r_{ij} is the magnitude of the distance between two arbitrary particles, $\mathbf{f}_{ij}$ is the force that atom j exerts on atom i , m is the atomic mass, $\mathbf{r}_i$ is the position of the particle i , $\mathbf{f}_i$ is the total force and N_m is the total number of particles in the simulation system. Herein, the 12-6 Lennard-Jones (LJ) pair-wise potential in previous works (Zhang et al., 2020) is used to model the interaction forces for argon-argon, silver-silver and argon-silver atoms

$$U(r_{ij}) = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right], \quad (3.2)$$

where ϵ is the well-depth of the Lennard-Jones potential and σ is the collision diameter. For argon and silver atoms, there are $\epsilon_{Ar-Ar} = 0.0104 \text{ eV}$, $\sigma_{Ar-Ar} = 3.405 \text{ \AA}$, $\epsilon_{Ag-Ag} = 0.4080 \text{ eV}$ and $\sigma_{Ag-Ag} = 2.551 \text{ \AA}$, respectively (Papanikolaou, 2017). ϵ_{Ar-Ag} and σ_{Ar-Ag} can be obtained from the Lorentz-Bertholot rule (Lorentz, 1881; Berthelot, 1898)

$$\epsilon_{Ar-Ag} = \sqrt{\epsilon_{Ar-Ar} \epsilon_{Ag-Ag}} = 0.0651 \text{ eV}, \quad (3.3a)$$

$$\sigma_{Ar-Ag} = \frac{\sigma_{Ar-Ar} + \sigma_{Ag-Ag}}{2} = 2.978 \text{ \AA}. \quad (3.3b)$$

In the following text, we vary ϵ_{Ar-Ag} with fixed σ_{Ar-Ag} to tune the wetting ability of the wall. For brevity, dimensionless ϵ_{Ar-Ag}^* defined as $\epsilon_{Ar-Ag}/\epsilon_{Ar-Ar}$ is applied. To reduce the computational cost, the Lennard-Jones potential

is truncated using a typical cut-off distance $r_c = 2.5\sigma$ (Rapaport, 2004). Interactions of two arbitrary atoms are not considered if the distance between them is greater than this cut-off value. Throughout this work, atoms' velocities are updated via the verlet algorithm and 1 fs is chosen as the time step. The first 0.5 ns is used to reach an equilibration phase in the NVT ensemble (Hoover, 1985) to thermally relax the MD system before applying artificial forces to drive liquid atoms flow and performing Langevin thermostat. The following 2.5 ns is for the MD system to achieve the steady state and then another 5 ns to collect data.

To drive liquid argon atoms to flow in the x direction, Markvoort et al. (Markvoort et al., 2005) artificially added a force f_x for each atom in the D_2 region after resetting the temperature T of atoms in domain D_1 to T_i to meet the inlet temperature boundary condition. However, this force may increase energies of atoms to drive their real temperatures to deviate from desired values, since the externally forced region is located upstream of the thermostat domain. Hence, the order of forcing and thermostat domains is changed herein. Every atom in D_1 moves in x direction driven by the external force f_x . Then, an average velocity u_a is subtracted from each atom's x velocity component before using the Langevin thermostat algorithm (Schneider and Stoll, 1978a) to control the temperature in D_2 .

3.1.2 Definition of physical quantities

The local dimensionless temperature of argon atoms is defined as

$$\theta_m(\xi) = \frac{T_m(\xi) - T_w}{T_i - T_w} \text{ with } T_m(\xi) = \frac{\int_0^1 c\rho u(\eta)T(\xi, \eta)d\eta}{\int_0^1 c\rho u(\eta)d\eta}, \quad (3.4)$$

where T_w and T_i are wall temperature and inlet temperature of liquid argon, respectively. ξ and η are dimensionless coordinates in streamwise and spanwise directions, respectively, defined as $\xi = x/(Pe \cdot H)$ and $\eta = y/H$.

As aforementioned, there can be velocity and temperature slip on the surface of the wall at the nanoscale. The velocity slip length (L_v) is related with the fluid behaviour including the slip flow magnitude and the potential effects of surface advection, and is given by

$$L_v = \frac{\Delta u_{wf}}{\left. \frac{\partial u}{\partial y} \right|_{y=H}}, \quad (3.5)$$

where Δu_{wf} is the difference between the wall velocity and the fluid velocity at the wall, and $\left. \frac{\partial u}{\partial y} \right|_{y=H}$ is the velocity gradient of fluid at the interface.

The thermal slip length (L_T) reveals the importance of discontinuity of fluids temperature at the wall, and can be written as

$$L_T = \frac{\Delta T_{wf}}{\left. \frac{\partial T}{\partial y} \right|_{y=H}}. \quad (3.6)$$

Similarly, ΔT_{wf} is the discrepancy between wall temperature and fluid temperature at the interface, and $\left. \frac{\partial T}{\partial y} \right|_{y=H}$ is the temperature gradient of argon at the wall.

Moreover, the local dynamic viscosity of liquid atoms can be evaluated from (Vo et al., 2015)

$$\mu = \frac{\tau_{xy}}{\dot{\gamma}}, \quad (3.7)$$

where τ_{xy} is the shear stress vector, and $\dot{\gamma}$ is the shear rate. For the planar Poiseuille flow, $\dot{\gamma} = du(x)/dy$, and τ_{xy} is determined by the method of planes (Todd et al., 1995).

3.1.3 Details of geometrical models

Table 3.1: Physical parameters for liquid argon at 100K.

Thermal conductivity	Dynamic viscosity ($Pa \cdot s$)	Specific heat [$J/(Kg \cdot K)$]
101.24×10^{-3} ^a	0.2×10^{-3} ^d	1.165×10^3 ^g
110.00×10^{-3} ^b	$(0.18 \pm 0.027) \times 10^{-3}$ ^{d,e}	1.156×10^3 ^h
102.70×10^{-3} ^c	0.194×10^{-3} ^f	

^a the thermal conductivity of liquid Argon at 100K from reference (Kim et al., 2008a).

^b the thermal conductivity of liquid Argon at 100K from reference (McGaughey and Kaviani, 2004).

^c the thermal conductivity of liquid Argon at 102.3K from reference (Borgelt et al., 1990).

^d the dynamic viscosity of liquid Argon at 100K from reference (Koplik et al., 1989).

^e the dynamic viscosity of liquid Argon at 100K from reference (Koplik et al., 1988).

^f the dynamic viscosity of liquid Argon at 100K from reference (Kim et al., 2010).

^g the specific heat of liquid Argon at constant pressure from reference (Gladun, 1971).

^h the specific heat of liquid Argon at constant pressure from reference (Rice, 1946).

The length of the channel is determined by the inverse Graetz number $\frac{1}{Gz} = \frac{L}{D_H Pe} = 0.4$ in order to ensure that the hydrodynamically developed laminar flow is achieved in the channel (Lahjomri and Oubarra, 1999; Marable et al., 2017). Further, considering the numerical terms introduced in D_1 and D_2 and the periodic boundary condition used in the streamwise direction which induces nonphysical phenomena around the outlet part of D_3 , these three sections will be discarded when collecting data samples, as similarly performed in references (Ge et al., 2015; Gu et al., 2016; Marable et al., 2017). Consequently, a larger inverse Graetz number which is proportional to the channel length is chosen

$$\frac{1}{Gz} = \frac{L}{D_H Pe} \approx 1, \quad (3.8)$$

where Pe is the Péclet number and $Pe = RePr = \rho c_p / \kappa$.

Another key input is the dimensionless density (ρ^*). We choose $\rho^* \approx 0.8$ and the initial temperature T_0 is set to 100K which corresponds to the liquid state of argon (Kim et al., 2010). The geometrical dimensions of the

channel and the number of argon atoms inside the channel should satisfy the following equation

$$\rho^* = \frac{N}{V} \sigma_{Ar-Ar}^3 = \frac{N}{LWH} \sigma_{Ar-Ar}^3 \approx 0.8. \quad (3.9)$$

Moreover, Haji-Sheikh et al. (Haji-Sheikh et al., 2008) and Haddout et al. (Haddout and Lahjomri, 2015) stressed that the axial conduction (see Eq. (2.4)) influence needs to be considered when the Péclet number (Pe) is less than 10 after applying the series analysis solution approach to study the temperature distributions in parallel plate channels or circular ducts, respectively. Further, Hennecke (Hennecke, 1968) stated that axial conduction might be neglected at $Pe > 20$. To fully clarify the limitation of analytical models in various situations, Pe within the following three intervals was tested in this work: $Pe_1 \in (0, 10)$, $Pe_2 \in (10, 20)$ and $Pe_3 \in (20, +\infty)$.

Table 3.2: Geometrical dimensions of the parallel plate channel and control parameters for $\epsilon_{Ar-Ag} = 0.0651 \text{ eV}$ and $\sigma_{Ar-Ag} = 2.978 \text{ \AA}$.

u_a (m/s)	$2H$ (nm)	L (nm)	W (nm)	T_w (K)	Pe	N_f	L_{D1} (nm)	L_{D2} (nm)
33.50	24	1069.2	3.2	150	24.874	1664021	1.2	2
33.50	24	1069.2	3.2	190	24.874	1664021	1.2	2
33.50	12	267.2	3.2	150	12.437	207924	1.6	1.6
33.50	12	267.2	3.2	190	12.437	207924	1.6	1.6
33.50	6	66.8	3.2	150	6.218	25990	1.6	1.6
33.50	6	66.8	3.2	190	6.218	25990	1.6	1.6

Similar to reference (Jeong and Jeong, 2006), physical parameters for the liquid argon are postulated as constant as shown in Table 3.1. Considering Eqs. (3.8) and (3.9), and the geometrical dimensions of the channel, the total number of fluid atoms and average velocities are selected (shown in Table 3.2 for clarity).

In the entire simulation process, the outmost silver atoms are frozen to their respective FCC lattice sites to prevent losing wall atoms, and the re-

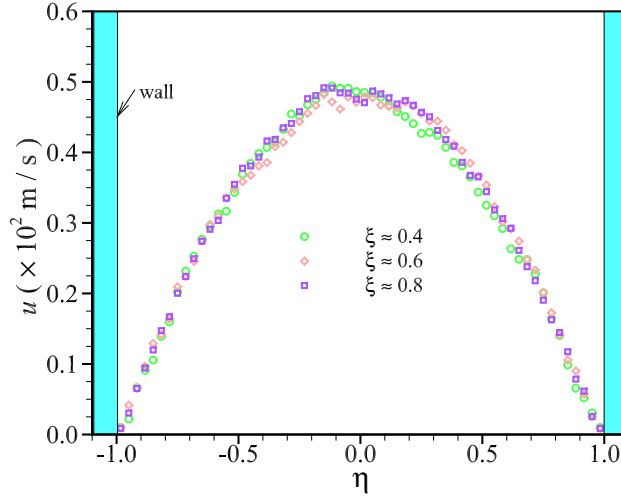
maintaining silver atoms are constrained to their initial lattice sites via using the virtual harmonic spring. This mimics wall atoms' real motions as it allows these particles to oscillate (Cieplak et al., 2001). The following factors should be considered when choosing the value of the spring constant: (1) maintaining well-defined wall boundary structures with a computationally acceptable number of particles; (2) ensuring that the distance between wall atoms is small enough to prevent fluid particles leaking through the wall (Powles et al., 1992); (3) preventing solid wall particles from being over-constrained during the process of molecular dynamics simulations (Cieplak et al., 2001). Based on these constraints, Thompson et al. (Thompson and Robbins, 1990) argued that this parameter can be evaluated according to the Lindemann criterion: $\langle \delta u^2 \rangle / d^2 < 0.023$. $\langle \delta u^2 \rangle$ is the mean squared displacement about the lattice site and d is the nearest-neighbour distance. However, it is complex to determine the spring constant through the Lindemann criterion as some parameters in this rule have to be obtained from neutron scattering experiments. Khare R et al. (Khare et al., 2006) proposed another straightforward method to estimate the spring constant

$$K_s = \frac{500\varepsilon}{\sigma^2}. \quad (3.10)$$

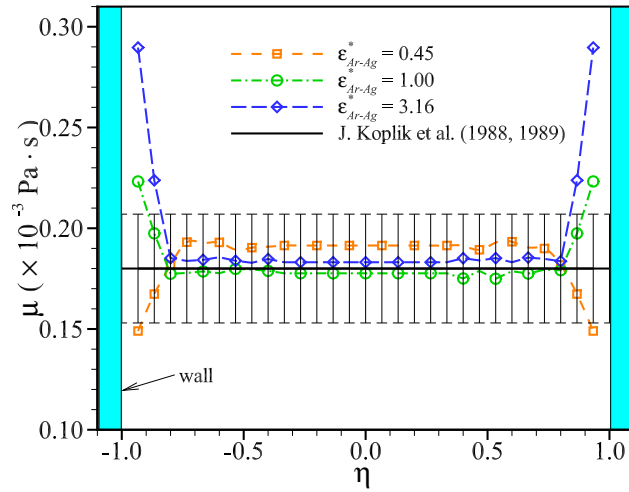
Based on this criteria, the spring constant is 502 N/m as will be used throughout this work.

3.1.4 Validation

The variation of streamwise velocity u on three cross sections ($\xi = 0.4, 0.6$ and 0.8) obtained from MD simulations is illustrated in Fig. 3.2. We can see that the velocity distribution is standard parabolic and velocities in the three cross sections are almost the same. Hence, flow in the plane


 Figure 3.2: Velocity profiles at $T_w = 190\text{ K}$ and $H = 12\text{ nm}$.

parallel channel driven by the approach introduced in Section 3.1.1 can be treated as hydrodynamically developed laminar flow (Markvoort et al., 2005; Ge et al., 2015; Gu et al., 2016; Marable et al., 2017). Moreover, one interesting observation is that there is no velocity slip (similarly, no velocity slip is observed for $H = 3$ or 6 nm , and the corresponding velocity profiles are not reported here for brevity). It will be illustrated later that this is owing to the large value of the energy parameter (ϵ_{Ar-Ag}) calculated from the Lorentz-Bertholot rule.


 Figure 3.3: Effects of wall wettability on the dynamic viscosity of the liquid argon at $H = 6\text{ nm}$, $T_w = 150\text{ K}$ and $u_a \approx 33.5\text{ m/s}$.

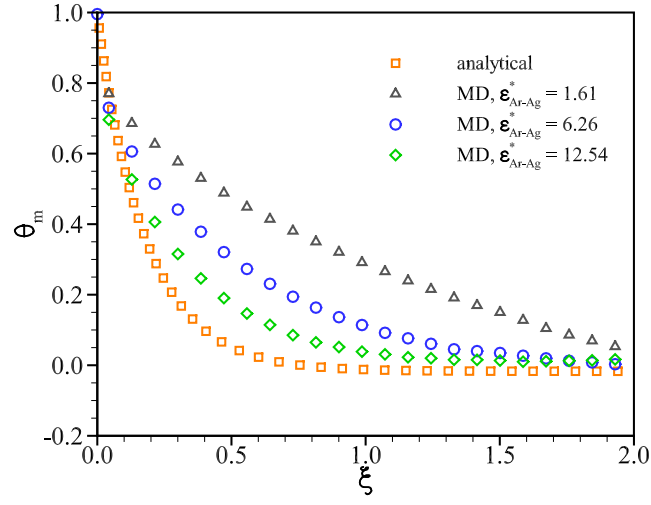
In addition, the local viscosity profiles are also calculated. As shown in Fig. 3.3, the bulk viscosity shows good agreement with experiment data marked by the black line (the relative error is less than 5%). However, the viscosity at the wall-fluid interface deviates from the bulk value, and exhibits an upward trend at larger wall-fluid interaction strength. These observations of the velocity and viscosity validate the correctness of the calculations in this work.

3.2 Limitation of the analytical model based on continuous assumptions

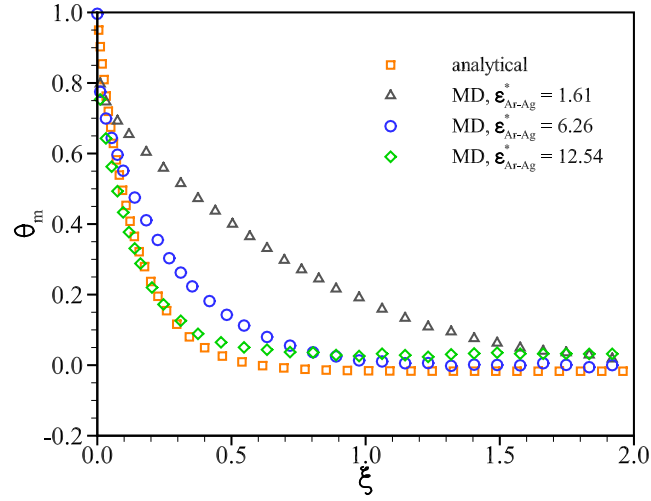
The continuum-based energy equation (see Section 2.1) becomes less valid when depicting nanoscale flow and heat transfer problems due to the violation of the no-slip boundary conditions, the non-uniform density profile, etc. The convective heat transfer in the nanoscale channel shown in Fig. 3.1 is explored by both the MD simulation and the energy equation.

The bulk non-dimensional temperature (θ_m) of liquid argon is shown in Fig. 3.4. Clearly, a higher energy parameter leads to lower dimensionless temperature over the thermally undeveloped region, but this effect vanishes when reaching the fully developed region. The analytical solution obtained by assuming the fluid dynamics is continuous and the density is constant (see Section 2.1) is also plotted. This analytical solution predicts well the temperature at high enough energy parameter but at low values of ξ , it underestimates the dimensionless temperature. When the channel becomes smaller, the discrepancy between the analytical and MD solutions also increases as the continuity assumption becomes less valid. These two parameters, ξ and H , will be further explored in the following section.

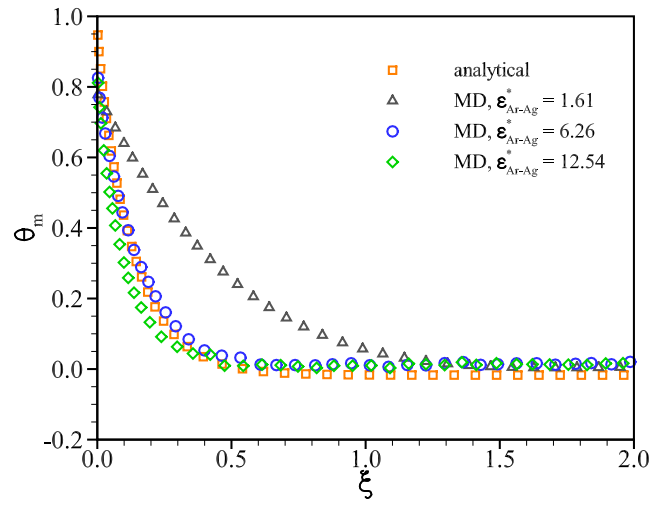
3.2. LIMITATION OF THE ANALYTICAL MODEL BASED ON CONTINUOUS ASSUMPTIONS



(a) $H = 3 \text{ nm}$



(b) $H = 6 \text{ nm}$



(c) $H = 12 \text{ nm}$

Figure 3.4: Dimensionless bulk temperature profile at mean velocity $u_a \approx 33.5 \text{ m/s}$ and $T_w = 190 \text{ K}$.

3.3 Results and discussions

The density oscillation, slip boundary conditions and viscosity variation are not accounted in the continuum based analytical model and are the significant features of the Micro/Nanoscale flow. Hence, the underlying physical mechanisms of the non-uniform density, slip, viscosity variation and their influences on the velocity and temperature profiles are examined by MD simulations in this section.

3.3.1 Density profile

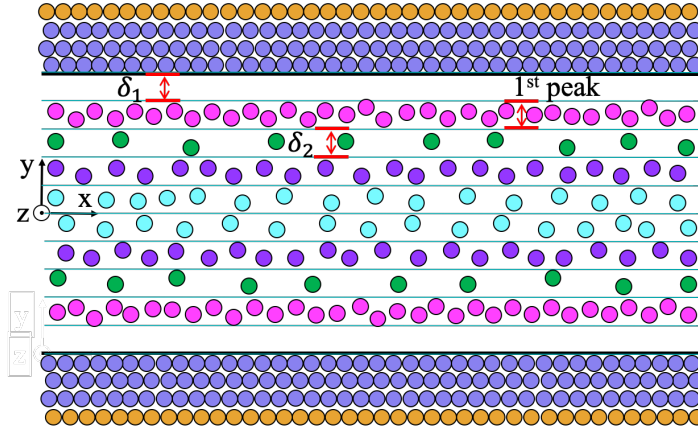


Figure 3.5: Density profile at mean velocity $u_a \approx 33.5 \text{ m/s}$, $T_w = 150 \text{ K}$, $H = 3 \text{ nm}$ and $\epsilon_{Ar-Ag}^* = 6.26$. Blue and brown circles represent wall atoms, and argon atoms are represented by other circles with different colors to clearly show the density layering phenomenon.

Fig. 3.5 schematically shows the density distribution obtained from MD simulations. Similar to reference (Yu et al., 2020), a clear stratification in the y direction can be observed and in the literature it has been linked to the oscillatory force curve (Bhushan et al., 1995) or the energy scale (Wang and Hadjiconstantinou, 2017). There are no liquid argon atoms in an extremely thin layer around $2\text{\AA}$ adjacent to the wall denoted as δ_1 in agreement with a previous observation that the thickness of the hollow layer

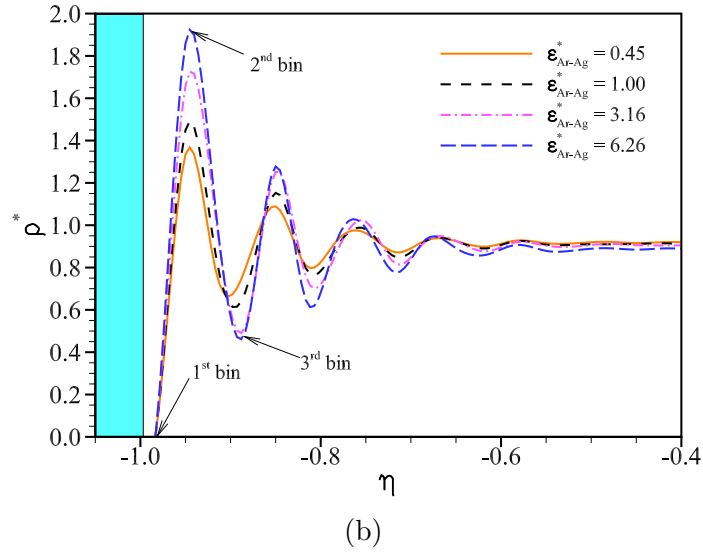
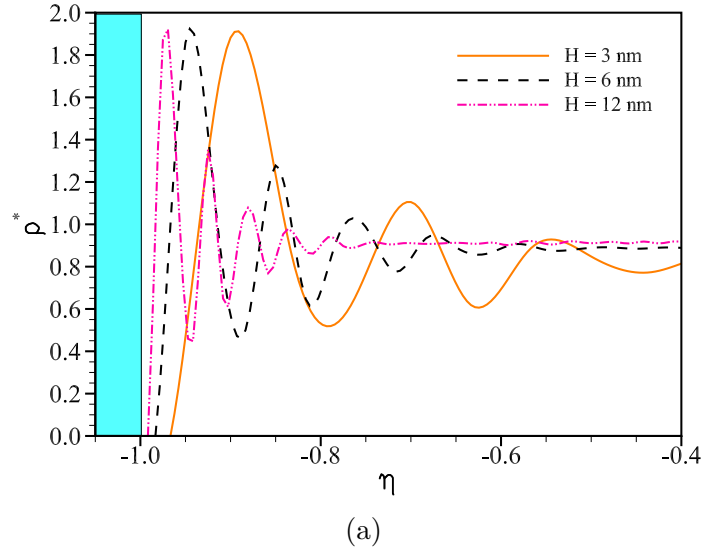


Figure 3.6: Dimensionless density ρ^* profile at the cross section with $\xi = 0.13$ for varying (a) channel height H ($u_a \approx 33.5 \text{ m/s}$, $\epsilon_{Ar-Ag}^* = 6.26$, and $T_w = 150 \text{ K}$) and (b) interaction strength ϵ_{Ar-Ag}^* ($u_a \approx 33.5 \text{ m/s}$, $T_w = 150 \text{ K}$, and $H = 6 \text{ nm}$).

is typically less than a nanometer (Huisman et al., 1997). Then, argon atoms form a high density layer followed by another low density region δ_2 . The further inwards layers are less notable and the profile becomes more uniform.

As the channel height results in strong differences between the MD and analytical solutions, its influence on the density profile is studied, as shown

in Fig. 3.6a. Results agree with the expectations that the length of the density fluctuation zone declines for increasing channel heights, confirming that the density fluctuation is only prominent in small scale channel flows. Fig. 3.6b shows that the dimensional density peak values increase with ϵ_{Ar-Ag}^* . However, the peak location of the density and the length of the density fluctuation region are almost unaffected by the wall wettability. In addition, the wall temperature has no significant effects on the density fluctuation profile over the parameters considered (the corresponding figure is not shown here for brevity).

One interesting observation is that the total number of argon atoms in the density layering region denoted as D_l in Fig. 3.7 at various ϵ_{Ar-Ag}^* is almost a constant value. The larger magnitude of oscillation at higher ϵ_{Ar-Ag}^* indicates some argon atoms move from the first and other bins to the second bin, as schematically shown in Fig. 3.7.

3.3.2 Velocity and thermal slip lengths

After clarifying the density layering phenomenon, the hydrodynamic and thermal slip lengths as another two factors causing the violation of the continuum-based model are then investigated based on the MD simulations to illustrate microscopic mechanisms.

Based on simulation results, the velocity slip length over the range of mean velocity studied ($27.2 \text{ m/s} \leq u_a \leq 100 \text{ m/s}$) is $0.61 \pm 0.046 \text{ nm}$, agreeing with that in reference (Thompson and Troian, 1997). Similarly, the thermal slip length is also observed to remain relatively constant at $9.34 \pm 1.185 \text{ nm}$ at various mean velocity, in agreement with reference (Marable et al., 2017).

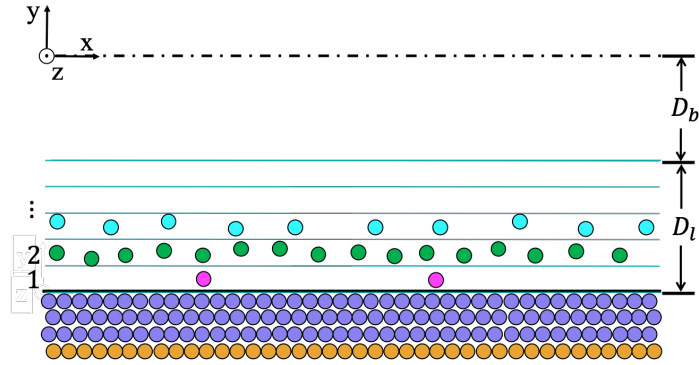
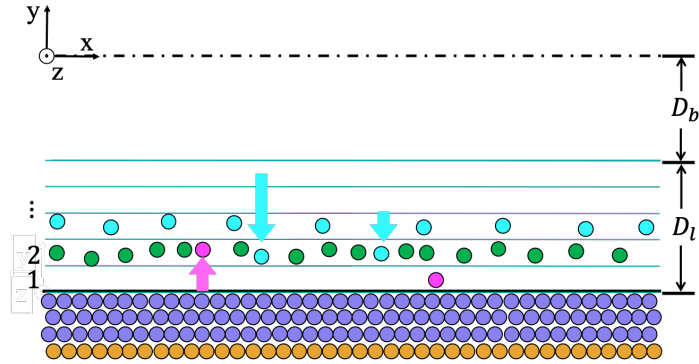
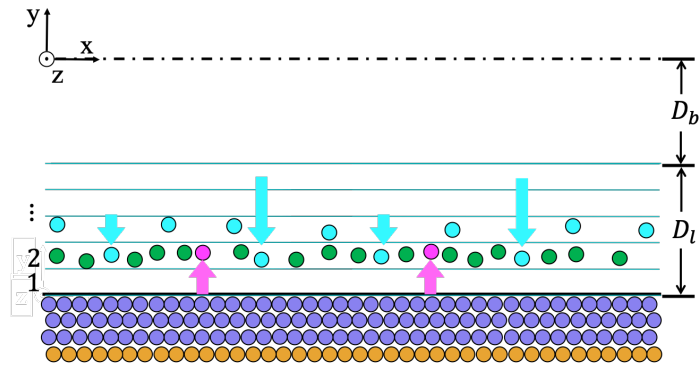
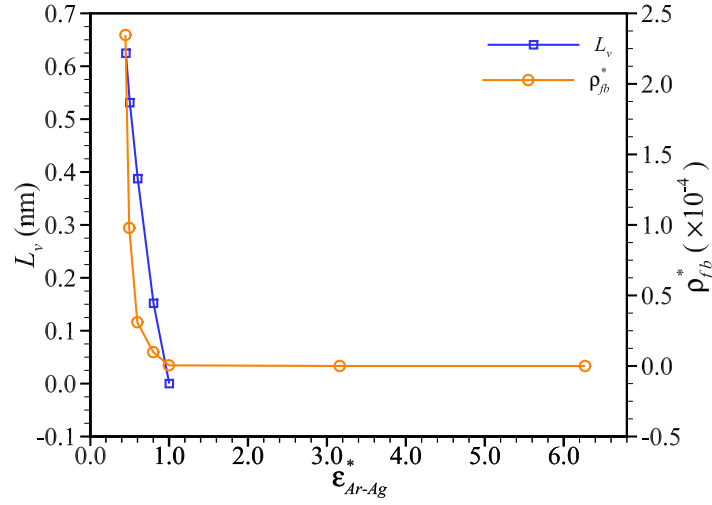
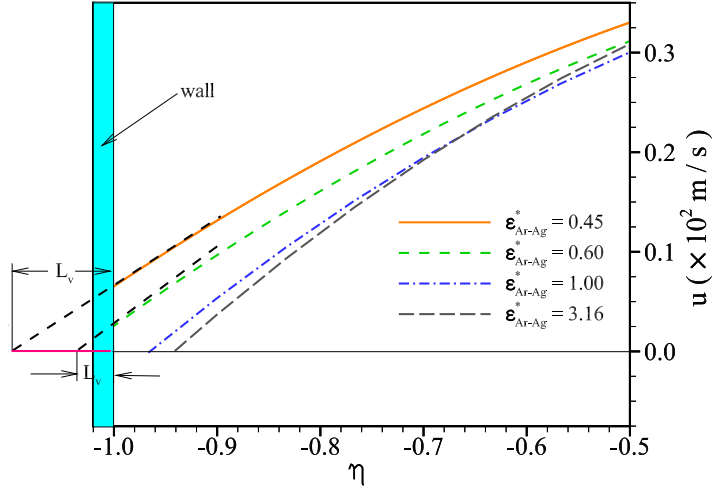

 (a) $\epsilon_{Ar-Ag}^* = 0.45$

 (b) $\epsilon_{Ar-Ag}^* = 1.00$

 (c) $\epsilon_{Ar-Ag}^* = 3.16$

Figure 3.7: Density profile in bins in the proximity of the wall at $H = 6 \text{ nm}$, $T_w = 150 \text{ K}$ and $u_a \approx 33.5 \text{ m/s}$. Only the lower part of the model is shown due to symmetry. Blue and brown circles represent wall atoms, and the other circles denote liquid argon atoms. D_b and D_l represent the density bulk and layering regions, respectively.



(a) Velocity slip length and density of argon in the first bin.



(b) Velocity profiles.

 Figure 3.8: Effects of wall wettability on the velocity slip length and density profile of the first bin at $H = 6 \text{ nm}$, $T_w = 150 \text{ K}$ and $u_a \approx 33.5 \text{ m/s}$.

Then, effects of the non-dimensional energy parameter ϵ_{Ar-Ag}^* in the LJ potential function characterising the wall wettability on the two slip lengths are studied. A significant decrease in velocity slip length from 0.62 to 0 nm is obtained by increasing the dimensionless energy parameter from $\epsilon_{Ar-Ag}^* = 0.45$ to $\epsilon_{Ar-Ag}^* = 1.00$ (a larger ϵ_{Ar-Ag}^* means a more hydrophilic wall), as can be seen in Fig. 3.8a. The reduction of L_v can also be observed intuitively from the velocity profile along the channel height direction in Fig. 3.8b. Meanwhile, one can find that the dimensionless density in the

first bin ρ_{fb}^* drops dramatically at larger ϵ_{Ar-Ag}^* and reaches 0 at $\epsilon_{Ar-Ag}^* \geq 3.16$. This indicates all liquid argon atoms are ejected from the hole region closest to the hydrophilic wall as schematically plotted in Fig. 3.7 and therefore no velocity slip phenomenon is observed.

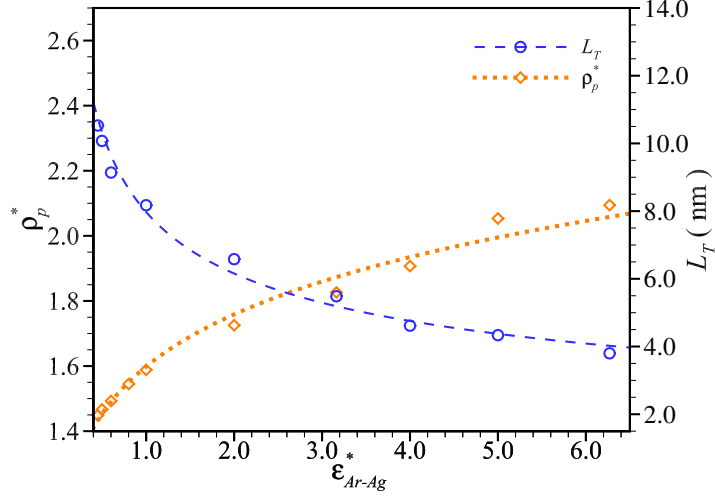


Figure 3.9: Effects of wall wettability on the temperature slip length and the first density peak of the liquid argon at $H = 6 \text{ nm}$, $T_w = 150 \text{ K}$ and $u_a \approx 33.5 \text{ m/s}$.

The effect of the liquid density layering on the thermal slip length (L_T) is further investigated as it is closely related to the layering or the density peak of liquid adjacent to the wall (Challis et al., 1961; Cahill et al., 2003; Alexeev et al., 2015). We again tune the wall wetting ability and the interfacial density profile of argon by adjusting ϵ_{Ar-Ag} with fixed σ_{Ar-Ag} for the LJ potential energy function. To quantify the difference of liquid argon density at various ϵ_{Ar-Ag}^* , a new variable is defined as

$$\rho_p^* = \frac{\rho_p}{\rho_b}, \quad (3.11)$$

where ρ_p is the first peak value of density and ρ_b is the bulk argon density far away from the interface. It is seen in Fig. 3.9 that L_T varies from 10.53 nm for a hydrophobic wall ($\epsilon_{Ar-Ag}^* = 0.45$) to 3.80 nm for a hydrophilic wall

($\epsilon_{Ar-Ag}^* = 6.26$). This observation aligns with previous reports (Kim et al., 2008a; Shenogina et al., 2009) that the wall wettability has a noticeable effect on L_T . Furthermore, the thermal slip length is found to be correlated with ρ_p^* : the higher the first density peak of liquid argon, the lower the thermal slip length. This coincides with the previous experiment result (Pollack, 1969) and molecular simulations (Alexeev et al., 2015) where water molecules confined by two graphene layers with different constant temperatures vibrate freely. However, the mechanism underpinning this correlation is unclear and further study is expected.

3.4 Conclusions

The liquid argon flow through a nanoscale channel is investigated by MD simulations and analytical modelling. The solution of the MD simulation deviates from the analytical one, which is based on the continuum assumption, as the height of the channel reduces. Then the nanoscale features violating this assumption are examined.

The density profile of argon atoms is found to exhibit a strong oscillation in the proximity of the fluid-wall interface named as the density layering regions, and then converges to the bulk value ($\rho^* \approx 0.8$) in the bulk domain further from the interface. The effect of wall wettability on ρ^* mainly concentrates on the density layering domain and the peak value of ρ^* next to the interface increases at the hydrophilic wall surface. The non-dimensional density layering region widens considerably at smaller channel height.

A dramatic reduction of the velocity slip length is observed when moving from hydrophobic to hydrophilic surfaces. For the super hydrophilic wall, the formation of a thin layer without liquid atoms impedes the velocity slip.

The thermal slip length is noticeably affected by the liquid argon atoms layering in the proximity of the wall and more specifically by the first peak value of argon atoms adjacent to the fluid-wall interface. Hence, the thermal slip length can be tuned via varying the wall wettability to change the first density peak value. These findings offer a new understanding of velocity and thermal slip at the interface, which can be applied to study the flow and heat dissipation at the nanoscale.

Chapter 4

Thermal and fluid flow in micro- and nano-scale channel with ice

In the last two chapters, the computational fluid dynamics (CFD) and molecular dynamics simulation are performed to investigate the effects of the velocity and temperature slips on the heat transfer and the flow resistance. Then, as a typical example of Micro/ Nanoscale heat transfer with phase change, the de-icing/ anti-icing with great importance is studied by molecular dynamics simulations to solve the outstanding issues as illustrated in Section [1.2.2](#).

4.1 Molecular dynamics simulation of thermal de-icing on a flat surface

4.1.1 Distinguishing of ice/water molecules

A critical challenge to apply the MD simulations to investigate the thermal de-icing process is the criterion to distinguish water and ice molecules. Mochizuki et al. (Mochizuki et al., 2013) identified the water molecules from the ice structure through evaluating if the molecule is “off-lattice”. Namely, an ice molecule was considered to become water if the distance between the particle and the nearest lattice point of the ice crystal with regular shape is more than 1 Å. Moore et al. (Moore et al., 2010) introduced the CHILL algorithm based on the local bond order parameter method (Rein ten Wolde et al., 1996). The coherence of molecules’ orientational order with that of their neighbours was employed to distinguish whether they belong to the crystal or liquid phase. Chau et al. (Chau and Hardwick, 1998) introduced the translational tetrahedral order S_k to measure the variation of the radial distances between the four nearest neighbor water oxygen atoms and the central water oxygen atom, and this parameter is defined as

$$S_k = 1 - \frac{1}{3} \sum_{k=1}^4 \frac{(r_k - \bar{r})^2}{4\bar{r}^2}, \quad (4.1)$$

where $\bar{r}$ is the arithmetic mean of the four radial distances, r_k is the radial distance from the k -th peripheral oxygen atom to the central oxygen atom. When the local tetrahedral order increases, S_k increases and even reaches a maximum value of 1 for a perfect tetrahedron. Compared with the tetrahedral order parameter introduced later, however, the translational tetrahedral order is much less used because it is more sensitive to the density fluctuation. Errington et al. (Errington and Debenedetti, 2001)

proposed the tetrahedral order parameter which was extensively applied to define ice-like and liquid-like molecules (Conde et al., 2008; Kumar et al., 2009; Pan et al., 2011; Martelli et al., 2018; Guardia et al., 2015), and the parameter was computed as

$$Q_i = 1 - \frac{3}{8} \sum_{j=1}^3 \sum_{k=j+1}^4 \left(\cos \theta_{j,i,k} + \frac{1}{3} \right)^2, \quad (4.2)$$

where i, j and k are indices for O atoms. The angle $\theta_{j,i,k}$ is formed by the O atoms of j, i and k (i is the vertex of the angle). Following Conde et al. (Conde et al., 2008), a molecule was classified as ice-like when $0.91 \leq Q_i \leq 1$. A wide range of order parameters used to characterize the local structure of liquid water/ice can be seen in previous work (Duboue-Dijonn and Laage, 2015). Also, the averaged hydrogen bonds for ice or water molecules are different. For example, the average hydrogen bonds for water molecules at 25 °C or ice molecules were estimated to 3.59 or 4.0, respectively (Jorgensen and Madura, 1985). Therefore, the time averaged value of the number of hydrogen bonds for each ice/water molecule is argued by Carignano et al. (Carignano et al., 2005), a reasonable physical quantity to identify the ice or water molecules. Although there are many definitions of the hydrogen bond such as the energetic definition through computing the potential energy of each pair of ice/water molecules (Starr et al., 1999), the electronic structure-based method and the geometric distance-angle definition (Kumar et al., 2007), the geometric distance-angle identification criterion is used for simplicity. In this method, two parameters, the cutoff angle (θ_{hb}) between the OH hydrogen bond and the OH covalent bond, and the cutoff distance (r_{hb}) between the O and H atoms at different molecules, should be defined appropriately. If the distance (r) between the H and O atoms on different molecules and the angle (θ) between water molecules meet the condition: $r \leq r_{hb}$ and $\theta \leq \theta_{hb}$,

a hydrogen bond is considered to be existing. Similar to reference (Kim and Yethiraj, 2008), r_{hb} and θ_{hb} are chosen as 3.5 Å and 40 °, respectively. In this work, both the averaged tetrahedral order parameter and hydrogen bonds for each ice/water molecule are applied to identify the water molecules from the ice.

4.1.2 Details of MD simulations

As depicted in Fig. 4.1a, hexagonal ice molecules (ice I_h) is investigated in this work because of its ubiquity in nature. The structure of ice I_h should follow the so-called "ice rules" (Bernal and Fowler, 1933): (1) there are two hydrogen atoms for each oxygen atom as the first neighbours; (2) each oxygen atom has two hydrogen atoms as the second neighbours; (3) there is only one hydrogen atom in the line joining two oxygen atoms. The pseudorandom ice configurations are generally generated based on the Cota and Hoover's method (Cota and Hoover, 1977) which is further developed in reference (Hayward and Reimers, 1997). A new straightforward method will be employed in this work to generate the ice I_h model. An ice I_h crystal should be download from the American Mineralogist Crystal Structure Database (AMCSD) (Downs and Hall-Wallace, 2003), and the ice model proposed in reference (Bernal and Fowler, 1933) is used. It should be noted that the hexagonal crystal system of ice crystal orientation as shown in Fig. 4.1 (a) should be rotated to the orthogonal crystal system via the AtomsK software. Then, the prescribed ice molecules can be built through expanding the ice crystal unit by the VESTA software (Momma and Izumi, 2008). Finally, the input data file for LAMMPS is generated by the VMD software (Humphrey et al., 1996).

For the silver wall whose cross-sectional area is $9.5 \times 9.5 \text{ nm}^2$, it is simulated

Table 4.1: Parameters for the TIP4P/ice potential.

Parameter	Values	Unit
m_H	1.008	g/mol
m_O	15.9994	g/mol
q_H	0.5897	e
q_O	-1.1794	e
r_0	0.9572	$\text{\AA}$
θ_0	104.52	$^\circ$
r_{OM}	0.1577	$\text{\AA}$
ϵ_{OO}	9.1427×10^{-3}	ev
σ_{OO}	3.1668	$\text{\AA}$
ϵ_{HH}	0	ev
σ_{HH}	0	$\text{\AA}$
ϵ_{OH}	0	ev
σ_{OH}	0	$\text{\AA}$
r_{cc}	8.5	$\text{\AA}$

with a face-centered cubic unit with a lattice constant of 0.4 nm . The wall model and Langevin thermostat in reference (Mao and Zhang, 2014) are employed to introduce physically-sound heat flux through the silver wall. Namely, the silver wall is divided into three sections. The bottom silver atoms marked in blue in Fig. 4.1b and Fig. 4.1c are fixed to prevent atoms from penetration, the red silver atoms are controlled by the aforementioned Langevin thermostat method to prescribed temperature and the cyan particles are “real” silver atoms which can vibrate freely. In total, there are 17150 atoms for the wall and 13104 – 137592 molecules of ice (at thickness $H = 4\text{ nm} - 16\text{ nm}$) considered in the simulation.

The freezing temperature of water predicted by the well-known SPC/E or TIP4P model is 215 K or 232 K , respectively (Abascal et al., 2005). The four-site water model (TIP4P/ice) in reference (Abascal et al., 2005) describes more accurately the near freezing point and bulk properties of the ice and water (see Table 4.1 for all parameters). For example, it predicts that the water freezing point is 272.2 K , very closer to the value of 273.15 K observed in experiments. Therefore, TIP4P/ice model is applied to model

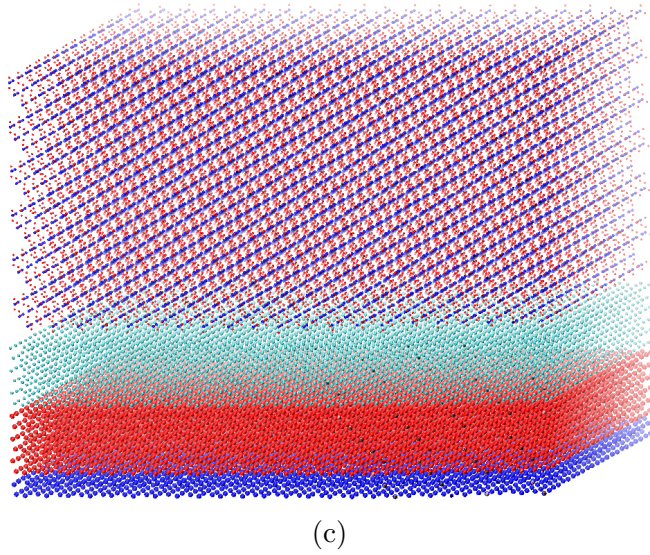
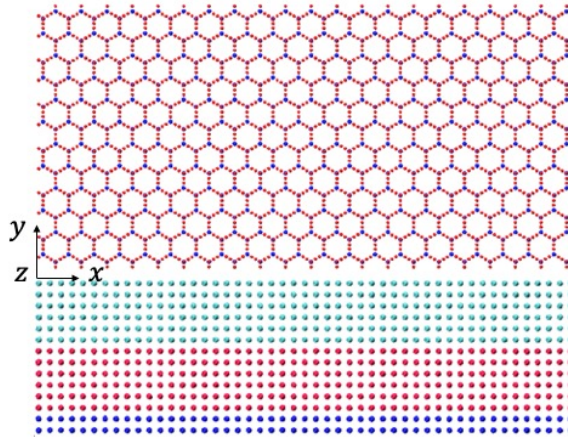
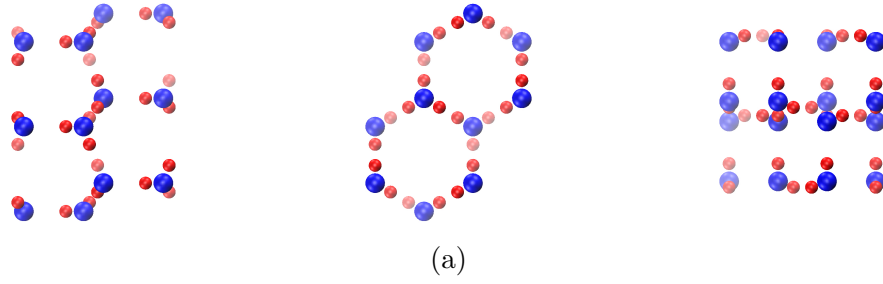


Figure 4.1: Sketch of the MD simulation system. (a) Ice I_h model from the side, front and top views. (b) and (c) show the ice-silver system from two-dimensional and three-dimensional views, respectively, and the cyan, red and blue particles below the ice are the three layers of silver atoms.

the ice and water in this work. A large time step of 1.0 *fs* in all simulation cases is enabled by adopting the SHAKE algorithm to constrain the bonds and angles of ice/water molecules, and the long-range electrostatic interactions are solved by employing the PPPM method (Andersen, 1983).

The interactions of silver atoms are described by the 12-6 Lennard-Jones (LJ) pair-wise potential proposed by Jones et al. (Jones, 1924):

$$U(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right], \quad (4.3)$$

where ϵ is the well-depth of the Lennard-Jones potential and σ is the collision diameter. $\epsilon_{Ag-Ag} = 0.4080 \text{ eV}$ and $\sigma_{Ag-Ag} = 2.551 \text{ \AA}$ respectively (Papanikolaou, 2017). Moreover, only the interactions between the silver and oxygen atoms in ice/water molecules are calculated, and the LJ potential is also used to compute the atomistic forces. ϵ_{Ag-O} and σ_{Ag-O} are determined from the Lorentz-Berthelot rule (Lorentz, 1881; Berthelot, 1898):

$$\epsilon_{Ag-O} = \sqrt{\epsilon_{Ag-Ag} \epsilon_{O-O}} = 0.0611 \text{ eV}, \quad (4.4a)$$

$$\sigma_{Ag-O} = \frac{\sigma_{Ag-Ag} + \sigma_{O-O}}{2} = 2.8589 \text{ \AA}. \quad (4.4b)$$

The Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package is used to perform all simulations. The periodic boundary conditions in all three directions are used throughout the work. It should be pointed out that a vacuum space with the same thickness from the top of the ice to the bottom of the silver substrate is added to the top of the ice to eliminate the interaction between the top ice atoms and the bottom substrate atoms resulting from the periodic boundary condition. Each case includes the following three steps: (1) the temperature of the ice-silver sys-

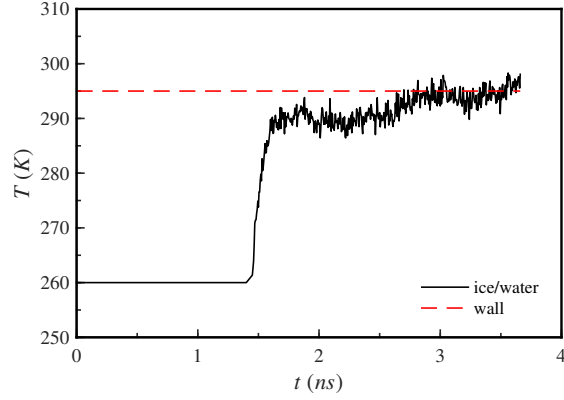
tem is adjusted to 260 K through the Langevin thermostat approach for 0.4 ns under the NVT ensemble to ensure that the equilibration state is achieved; (2) silver atoms shown in red are then heated to a given temperature while maintaining the ice temperature at 260 K through applying the Langevin thermostat (wall atoms marked in cyan oscillate freely) and (3) the thermostat algorithm is then removed from ice molecules to melt the ice by the hot wall.

Table 4.2: The average number of hydrogen bonds and tetrahedral order parameters $\langle Q \rangle$ for each ice/water molecule at various temperature.

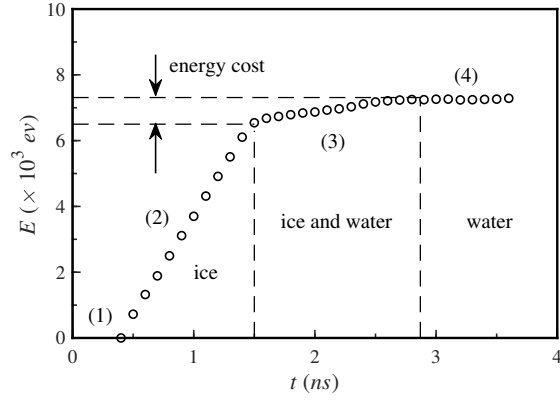
			reference value	present work	relative error
Hydrogen bonds	ice		4 (Jorgensen and Madura, 1985)	3.99	0.25%
		273.15 K	3.69	3.77	2.17%
		298.15 K	3.59	3.66	1.95%
	water	333.15 K	3.41	3.51	2.93%
		373.15 K	3.24	3.33	2.78%
$\langle Q \rangle$	ice		1 (Errington and Debenedetti, 2001)	0.95	5.00%
	water	295 K	0.70 (Martelli et al., 2018) or 0.678 (Guardia et al., 2015)	0.69	1.43% or 1.77%

To validate the accuracy of this work, the average number of hydrogen bonds and tetrahedral order parameters ($\langle Q \rangle = (1/N) \sum_i^N Q_i$, where N is the total number of O atoms (Kumar et al., 2009)) for each ice/water molecule are computed by our Tool Command Language (TCL) script, and the results are summarized in Table 4.2. One can observe that the maximum relative error between our results and the reference is less than 5%. The result also validates the TCL code that will be used to visualize the thermal de-icing process in Section 4.1.4.

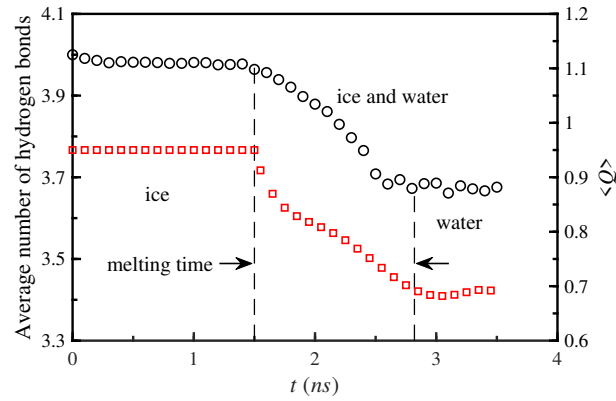
4.1. MOLECULAR DYNAMICS SIMULATION OF THERMAL DE-ICING ON A FLAT SURFACE



(a)

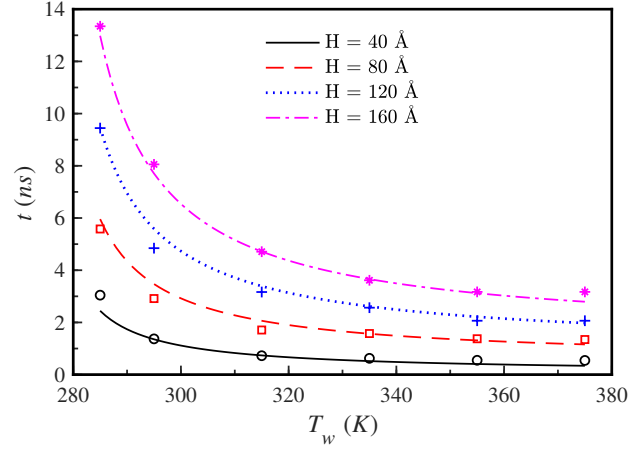


(b)

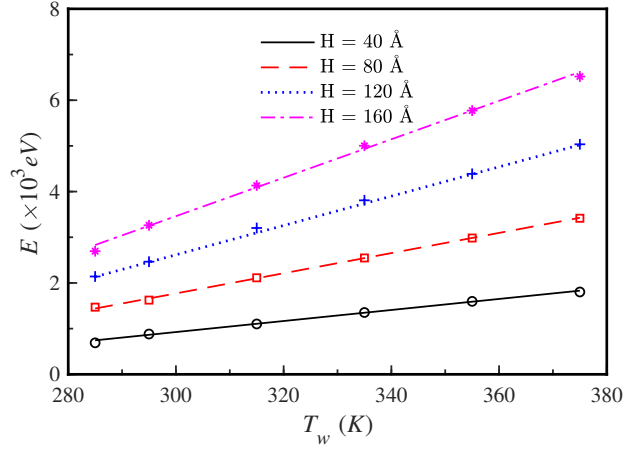


(c)

Figure 4.2: (a) Temperature (T), (b) energy input (E) and (c) the average number of hydrogen bonds and the tetrahedral order parameter per ice/water molecule during the thermal de-icing process at $T_w = 295\text{ K}$, $H = 40\text{ \AA}$, $\epsilon_{Ag-O} = 0.0611\text{ eV}$ and $\sigma_{Ag-O} = 2.8589\text{ \AA}$, respectively.



(a)



(b)

Figure 4.3: (a) De-icing time and (b) energy cost at various thickness and wall temperature with $\epsilon_{Ag-O} = 0.0611 \text{ eV}$. Curves and scatter points are computed from fitting equations shown in Eq. (4.5) and simulation results, respectively.

4.1.3 Effects of ice thickness, wall temperature and wettability on thermal de-icing

The thermal de-icing on the silver surface is studied by following the three MD simulation steps illustrated in Section 4.1.2. As shown in Fig. 4.2a, the initial temperature of ice and silver wall is artificially modulated to 260 K and 295 K , respectively, via the Langevin thermostat. Within a very short

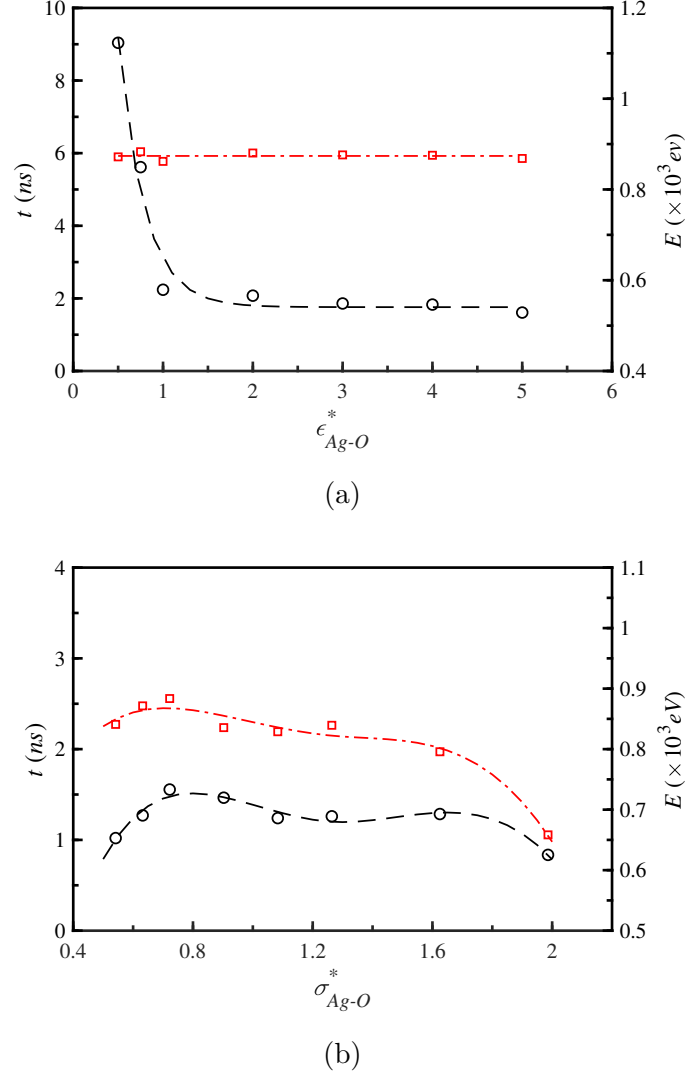


Figure 4.4: Energy cost and de-icing time at various ϵ_{Ag-O}^* and σ_{Ag-O}^* . (a) $\sigma_{Ag-O} = 2.8589 \text{ \AA}$, $H = 40 \text{ \AA}$ and $T_w = 295 \text{ K}$. (b) $\epsilon_{Ag-O} = 0.0611 \text{ eV}$, $H = 40 \text{ \AA}$ and $T_w = 295 \text{ K}$. Red dash-dotted line and black dash line represent the energy cost and melting time, respectively. Curves and scatter points are fitting and simulation results, respectively.

time after the thermal de-icing process starts, the ice/water temperature jumps to around 290 K , and then increases mildly to the wall temperature. One should note that the oscillation of ice/water temperature as seen in Fig. 4.2a is caused by the thermal fluctuations of ice/water molecules.

The cumulative energy input applied to heat the wall is displayed in Fig. 4.2b, which is a constant value at the equilibrium state or the state where all

ice molecules are melted. This validates the rationality of the simulation setup. The energy cost at stage (2) is used to heat “real” silver atoms before melting ice. The energy consumption during the thermal de-icing process is then defined as the difference of the cumulative energy at stage (2) and (4).

With the melting of ice, the number of averaged hydrogen bonds and the tetrahedral order parameter shown in Fig. 4.2c decrease gradually in good agreement, and the time consumption is then defined as the melting time.

Comparing Fig. 4.2a and Fig. 4.2c, the averaged number of hydrogen bonds for each water/ice molecule is found to be around 4.0 at the time when the ice temperature increases suddenly. This indicates that the thermal melting process can be roughly divided into two stages: ice temperature rises rapidly approximately to wall temperature, and then ice starts to melt gradually. Further details on the melting snapshots will be clarified later.

The thermal de-icing at various thickness and wall temperature is then investigated, and the result is shown in Fig. 4.3. At a higher temperature, for example, $T_w = 375\text{ K}$, the ice I_h crystal collapses as soon as it is heated. The fast thermal de-icing process for the case of high wall temperature is in agreement with previous observations (Mochizuki et al., 2013). Besides, the melting time decreases sharply to almost a constant value at $T_w \geq 313.15\text{ K}$ while the corresponding energy cost almost increases linearly. Hence, it is unnecessary to adopt higher wall temperatures during the practical design and applications, as also reported in reference (Wang et al., 2008). The thermal de-icing time and energy consumption shown in Fig. 4.3 can be approximated by the following equations with a root mean square error

less than 1%:

$$t(T_w, H) = \frac{9.033H - 7.903}{T_w - 273.15} + 0.1158H - 0.4005, \quad (4.5a)$$

$$E(T_w, H) = (2.5H + 2.078)T_w - 538.6H - 543.9, \quad (4.5b)$$

where the units for t , T_w , H and E are ns , K , nm and ev , respectively. These formula suggest that the melting time is a bilinear function of H and $T_w - 273.15K$ while the energy consumption is bilinear to H and T_w .

According to previous studies, the wettability of a solid wall is also an important factor affecting the accumulation of ice. Therefore, we change the interaction strength ($\epsilon_{Ag-O}^* = \epsilon_{Ag-O}/\epsilon_{O-O}$, a larger ϵ_{Ag-O}^* means a hydrophilic wall surface) while fixing the wall temperature as $295 K$ to examine the effects of this parameter on thermal de-icing, and the result is shown in Fig. 4.4. The energy consumption is almost independent on wall wettability. The melting time reduces at a larger ϵ_{Ag-O}^* , and can be approximated as

$$t(\epsilon_{Ag-O}^*) = 7.48 \exp(-3.435\epsilon_{Ag-O}^* + 1.711) + 1.759. \quad (4.6)$$

This observation indicates that more time is required to melt the ice accreted on the hydrophobic surface although such a surface is generally considered as the anti-icing material (Xiao et al., 2019; Bao et al., 2018). Similarly, the collision diameter ($\sigma_{Ag-O}^* = \sigma_{Ag-O}/\sigma_{O-O}$) is also varied, and the corresponding melting time and energy consumption increase firstly and then decrease (see Fig. 4.4b).

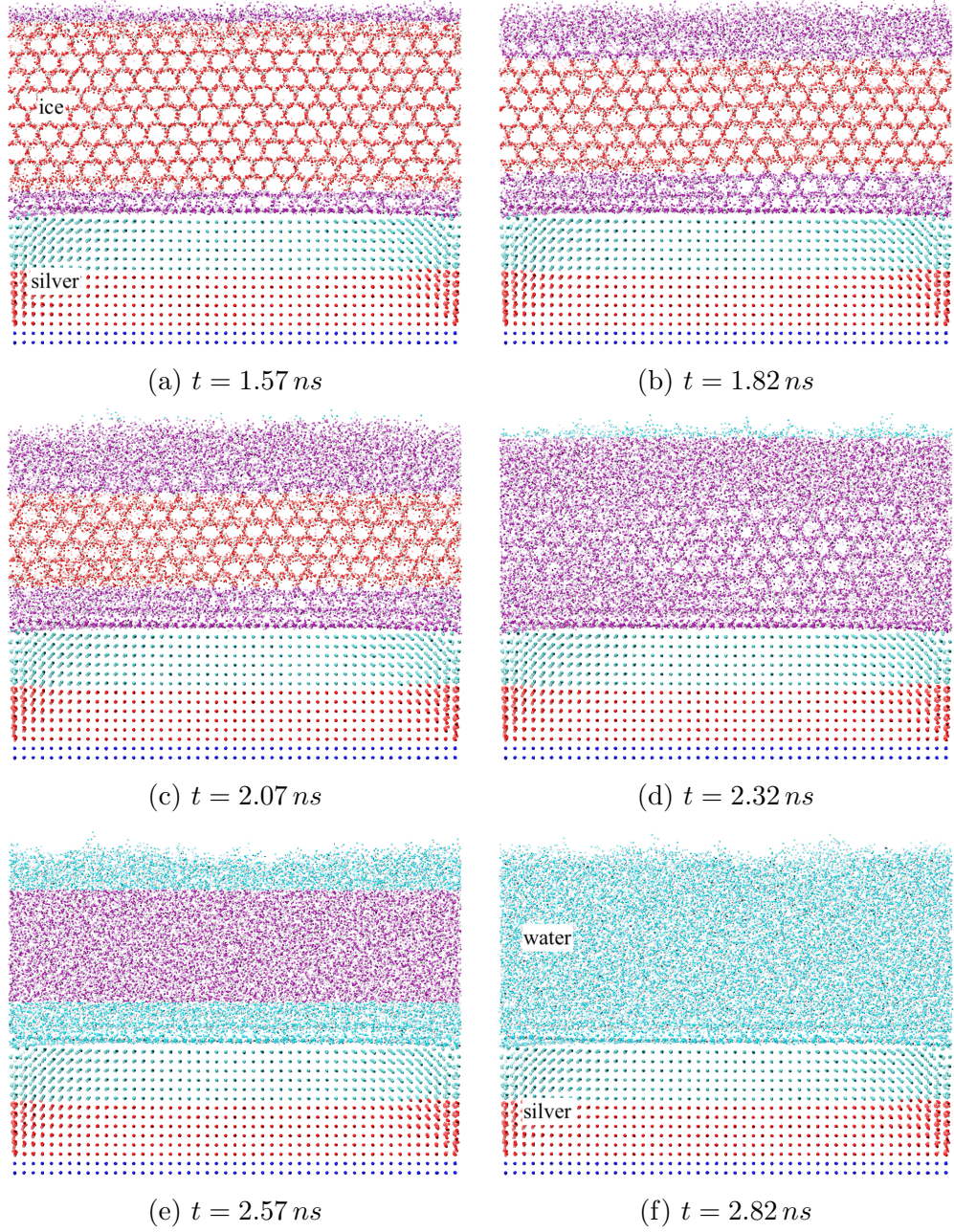


Figure 4.5: Snapshots of thermal de-icing at $T_w = 295 \text{ K}$, $H = 40 \text{ \AA}$, $\epsilon_{Ag-O} = 0.0611 \text{ eV}$ and $\sigma_{Ag-O} = 2.8589 \text{ \AA}$. The shallow blue or red particles denote the water or ice molecules, respectively, and the purple one is the phase between ice and water.

4.1.4 Physics of the thermal de-icing

In Section 4.1.3, we have illustrated the effects of wall temperature and wettability and the thickness of ice on the thermal de-icing time and energy consumption. The physical details during the process of thermal de-icing

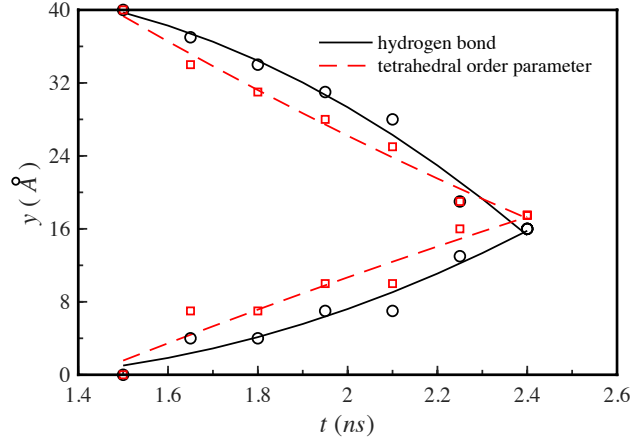


Figure 4.6: The profile of the melting front location (namely, the interface between the ice and quasi-liquid layer) at $T_w = 295\text{ K}$, $H = 40\text{ Å}$, $\epsilon_{Ag-O} = 0.0611\text{ eV}$ and $\sigma_{Ag-O} = 2.8589\text{ Å}$. Curves and scatter points are fitting and simulation results, respectively.

will be examined in this section.

Here, the case with $T_w = 295\text{ K}$, $H = 4$ and $\epsilon_{Ag-O} = 0.0611\text{ eV}$ is considered as an example to show the thermal de-icing process (the de-icing processes at other combinations of parameters are similar, and are not presented for brevity). The ice structure is divided into 10 bins with a height of 0.4 nm along the wall-normal direction. The average number of hydrogen bonds for each ice/water molecule is then computed by the aforementioned TCL script for each bin at a prescribed time step. Based on this method, the melting snapshots are then displayed in Fig. 4.5. One can observe that there is a quasi-liquid layer between the ice and the silver wall at the beginning of the thermal de-icing process, and this observation coincides with previous studies (Engemann et al., 2004; Sánchez et al., 2017). Besides, an interesting observation, which is independent of the thickness of ice layer, is that the ice begins to melt from the top and the bottom surfaces, and proceeds inwards, as shown in Fig. 4.6. This is in agreement with the previous investigations where the local bond order parameter method was employed

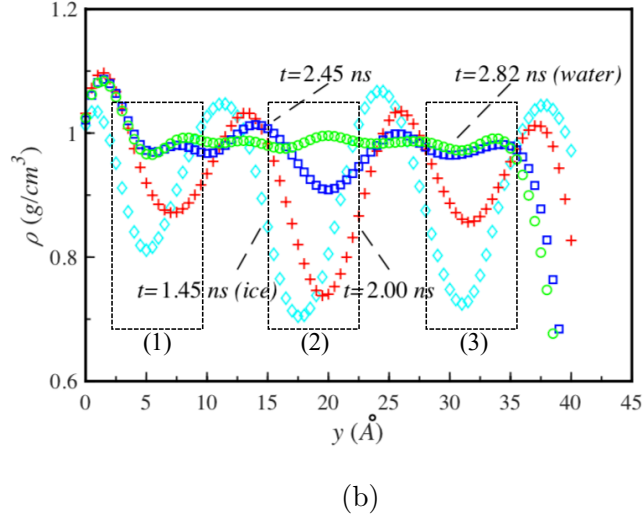
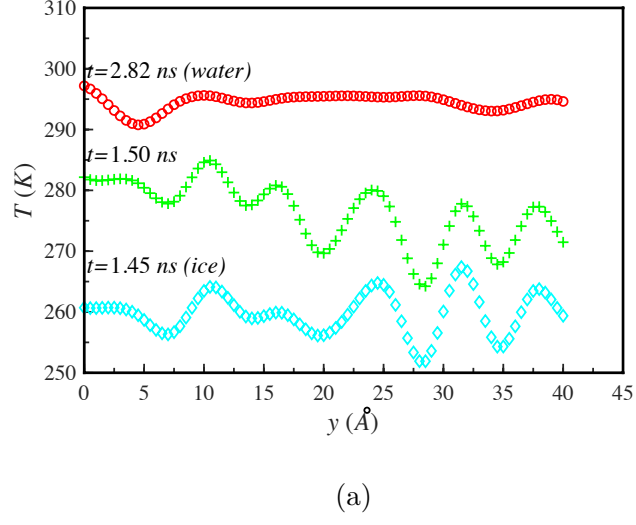


Figure 4.7: (a) and (b): Ice/water temperature and density profiles during the thermal de-icing process at $T_w = 295$ K, $H = 4$ nm and $\epsilon_{Ag-O} = 0.0611$ eV.

to distinguish ice and water molecules (Weber and Stillinger, 1983; Kroes, 1992; Sánchez et al., 2017).

It is worth noting that this thermal de-icing process is not caused by the periodic boundary conditions imposed in the simulations. To validate, the temperature distributions for four bins are sampled. If the outer-to-center thermal de-icing process is caused by the simulation setup of periodic boundary conditions, the temperature of the top and bottom ice bin should be equal to each other, and are higher than the temperature for middle ice

bins, which is obviously against the simulation results shown in Fig. 4.7a. Particularly, the temperature decreases with fluctuations along the y direction when melting ice (i.e., $t = 1.50\text{ ns}$), which indicates the heat flux flows from the bottom of ice to the top. Based on the explanation of Weber et al. (Weber and Stillinger, 1983), the de-icing process from the ice mantle to the core is caused by the ice structure. Ice molecules in the bulk are firmly fixed at their corresponding locations by a strongly directional tetrad of hydrogen bonds. However, the outermost ice molecules do not have enough hydrogen bonds, and then they move inwards to form extra hydrogen bonds, which will cause extra strains and disruption of initial network of the ice hydrogen bonds.

The density of ice/water is displayed in Fig. 4.7b. The ice density profile shows regular oscillation resembling the result reported in previous investigations (Sánchez et al., 2017; Conde et al., 2008). When the melting occurs gradually, the density of ice/water then gradually reduces to a steady value of 0.987 g/cm^3 , this is in excellent agreement with the reference value of 0.997 g/cm^3 . An interesting observation is that the local density for the top or bottom ice (see (1) and (3) marked in Fig. 4.7b) increases much faster than that of the middle of ice (see (2)). For example, local density for bin (1) or (3) is almost equal to the density of water while the density for the bin (2) is obviously less than the water density at $t = 2.45\text{ ns}$. This is one of the direct evidence that the melting process begins from the ice mantle and then proceeds inwards. Meanwhile, one can also observe that the bulk density of ice is less than that of the water, which is due to the ice crystal structure stabilized by hydrogen bonds.

4.2 Reduction of atomistic ice tensile stress by graphene-carbon nanotube coating

An interesting observation is that one-layer of graphene sheet with the atomistic smooth surface is an excellent icephobic coating, which can reduce the ice adhesion stress more than 200 MPa due to the hydrophobicity of the material (Xiao et al., 2016). Besides, the Van der Waals force is negligible if the distance between two particles is larger than 1.0 nm . Inspired by these two observations, we postulate that the three dimensional graphene-carbon nanotube junction (G-CNTs, see previous efforts (Zhu et al., 2012; Yan et al., 2013) for the synthesization method of such structure) sketched in Fig. 4.10d can be sandwiched between the ice and wall to reduce the ice tensile stress. For ice accumulating on the wall surface coated by G-CNTs, the ice adhesion force is then mainly contributed by the G-CNTs, more specifically, one-layer of a graphene sheet and some carbon atoms of carbon nanotubes on the C-CNTs (see carbon atoms marked in green in Fig. 4.16) when the distance between two graphene sheets is adjusted to be larger than 1.0 nm . Then, typical hydrophobic (i.e., silicon) and hydrophilic (i.e., silver and copper) wall substrate materials extensively applied in MD simulations are adopted to fully examine the effects of the primarily proposed multi-layers of graphene sheet and the G-CNTs on reducing ice tensile stress at the molecular level. Further, a water lubrication layer is added between the ice and substrate. This is motivated by the fact that the water lubricating layer has a positive effect on reducing the ice adhesion as reported in an experimental work (Lv et al., 2014). The resultant ice tensile stresses are then compared with each other results to determine the most efficient method of lowering the ice adhesion stress. Also, the impact of the free vibration of graphene coating on the ice adhe-

sion characteristics is explored because an absolute smooth graphene sheet reported in reference (Xiao et al., 2016) is not structurally stable due to the buckling phenomenon (Fasolino et al., 2007; Chen et al., 2014).

4.2.1 Details of geometric model

Three substrates including silver, copper and silicon are studied, and the simulation systems are summarized in Fig. 4.10 by using the silver substrate as an example. The ice I_h (hexagonal ice crystal, see Fig. 4.10a), is explored through the work because of its ubiquity in the biosphere (Lobban et al., 1998) although there are 18 phases of ice observed in experiments and nature (Klotz et al., 1999). To eliminate the size effect of the simulation system on the ice adhesion stress, four ice-silver systems (i.e., $A = 3.5 \times 3.5$, 6.5×6.5 , 9.5×9.5 and $12.5 \times 12.5 \text{ nm}^2$) are examined, and the result is shown in Fig. 4.8. To balance the accuracy of simulation results and the computational cost, the area of the ice $A = 9.5 \times 9.5 \text{ nm}^2$ with a thickness of 3.0 nm adhering to the substrates is adopted. The cross-sectional areas of the aforementioned three substrates and coating materials including multi-layers of the graphene sheet and G-CNTs consisting of electrically neutral atoms are equal to the area of the ice. The thickness of all substrates is 2.4 nm , and the distance between two arbitrary graphene layers is 0.335 nm . The carbon-carbon bond length in the carbon nanotube (CNT) or graphene is 0.1418 nm . Two layers of graphene are shown here for brevity although various number of layers sandwiched between ice and the silver substrate are investigated. For the G-CNTs structure, two graphene layers are connected by carbon nanotubes, and the number of CNT will also be adjusted to examine its effect on the ice adhesion stress.

For the method to generate the G-CNTs junction, Chen et al. (Chen

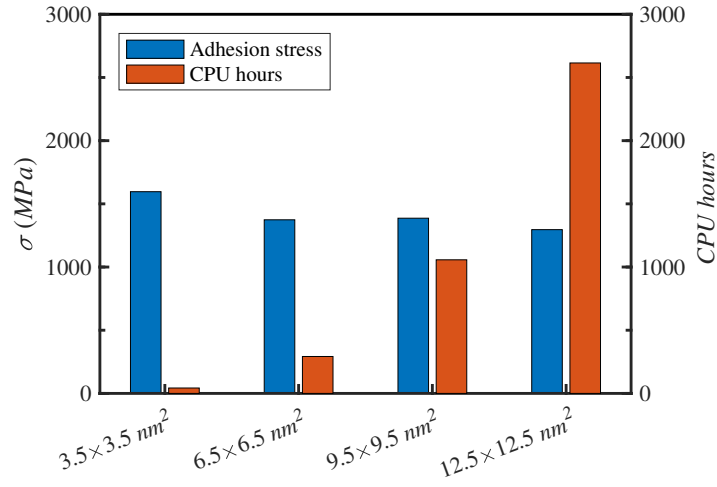


Figure 4.8: Ice adhesion stress and computational time for ice-silver simulation system of various areas.

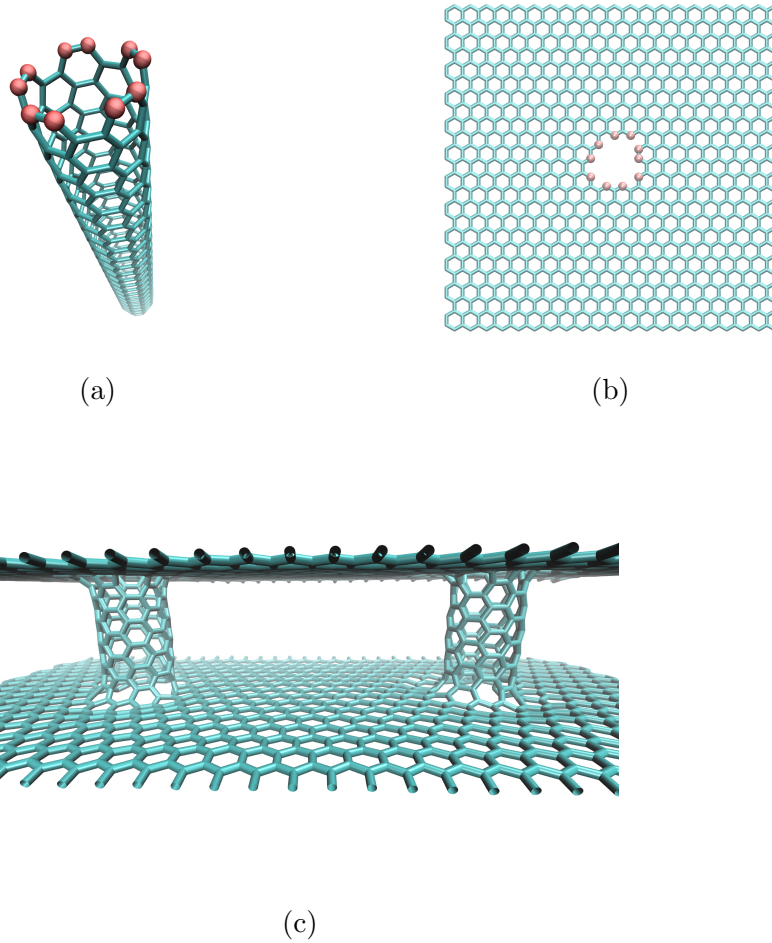


Figure 4.9: Sketch of G-CNTs system. (a) CNT (5, 5). (b) One-layer graphene with a pore. (c) G-CNTs structure.

et al., 2015) reported a straightforward approach to seamlessly connect CNTs with graphene via sp^2 covalent bonding. CNTs are placed between two graphene layers where some carbon atoms near CNTs are deleted according to the Euler's rule for polygons (Dimitrakakis et al., 2008). Axes of CNTs normal to graphene surfaces, and very small distances in the axial direction are preset between CNT ends and graphene layers. Then, the G-CNT junction structure can be automatically achieved by the relaxation process. It should be pointed out that the arbitrary presupposition distance is difficult to determine reasonably. Besides, Baowan et al. (Baowan et al., 2007) used the energy minimization method to produce such an atomic structure. However, many possible fusions of carbon nanotube and graphene have to be chosen manually, which is extremely inconvenient when the size of CNT is large. Therefore, the coupling approach (Zhang et al., 2018) including a pathfinding algorithm and the least-square method compensates the drawback in reference (Baowan et al., 2007), which is applied in this work to fabricate the atomic model of G-CNTs through three steps.

The first step is to delete some carbon atoms on the graphene to lead that the number of the dangling bonds on the graphene sheet is equal to that of a prescribed CNT through the pathfinding algorithm. In terms of a CNT (n, m) where n and m determine its configuration, $n+m$ dangling bonds can be observed at its one end. Then, a polygon with $n + m$ vertexes on the graphene sheet is determined by the pathfinding algorithm, and carbon atoms enclosed by the polygon are removed. For example, as shown in Fig. 4.9a and Fig. 4.9b, there are 10 dangling bonds marked with pink balls for CNT $(5, 5)$, and a polygon with 10 pink vertexes is obtained.

The second step is to minimize the bonding energy of the configuration determined in the first step to obtain a stable junction. The equation of

the bonding energy is formulated as

$$f(\Delta x, \Delta y, \Delta z, \Delta \theta) = \sum_{i=1}^N (|\mathbf{a}_i - \mathbf{b}_i| - \sigma)^2 \quad (4.7)$$

where $(\Delta x, \Delta y)$ is the moving vector of the graphene sheet located at the $z = 0$ plane, and Δz is the translation displacement of the CNT in z direction, $\Delta \theta$ is rotation angle of CNT along its axis, N is the number of carbon atoms, and σ is the carbon-carbon bond length. $\mathbf{a}_i$ and $\mathbf{b}_i$ are the positions of atoms on graphene sheet and CNT, respectively. Then, the least-square method is used to solve this equation and obtain the optimising G-CNTs junction. Finally, the equilibrium molecular dynamics (EMD) simulations with the isothermal-isobaric (NPT) ensemble is conducted to examine the thermodynamic stability of the generated junction. Similar to reference (Chen et al., 2015), the optimized Tersoff potential (Lindsay and Broido, 2010) is applied to depict the covalent bonding effect for the CNT and graphene, where the Lennard-Jones (LJ) potential is adopted to model the non-covalent interaction of CNTs (see reference (Girifalco et al., 2000) for parameters for this potential function model). The periodic boundary conditions are used for all three directions, and two vacuum domains with thickness around 5 nm are artificially added to the top or the bottom of the upper and lower graphene sheets to eliminate the interaction of the two graphene layers connected by CNTs. After the thermal relaxation process, the carbon atoms in the two graphene sheets close to CNTs are slightly lifted to connect with atoms at the end of CNTs, and then the seamless connected G-CNTs junction is obtained, as shown in Fig. 4.9c.

Here, the thickness of the water lubrication layer sandwiched between the ice and substrate is 1.0 nm (Hynninen et al., 2010). The ice is initially located on the top of the substrate with or without coating as close as

4.2. REDUCTION OF ATOMISTIC ICE TENSILE STRESS BY GRAPHENE-CARBON NANOTUBE COATING

possible without atomic overlap, and the distance between them is then automatically adjusted to form a stable structure through the equilibration simulation process illustrated in the following subsection. The number of atoms varies from 36000 to 84000, depending on the simulation system.

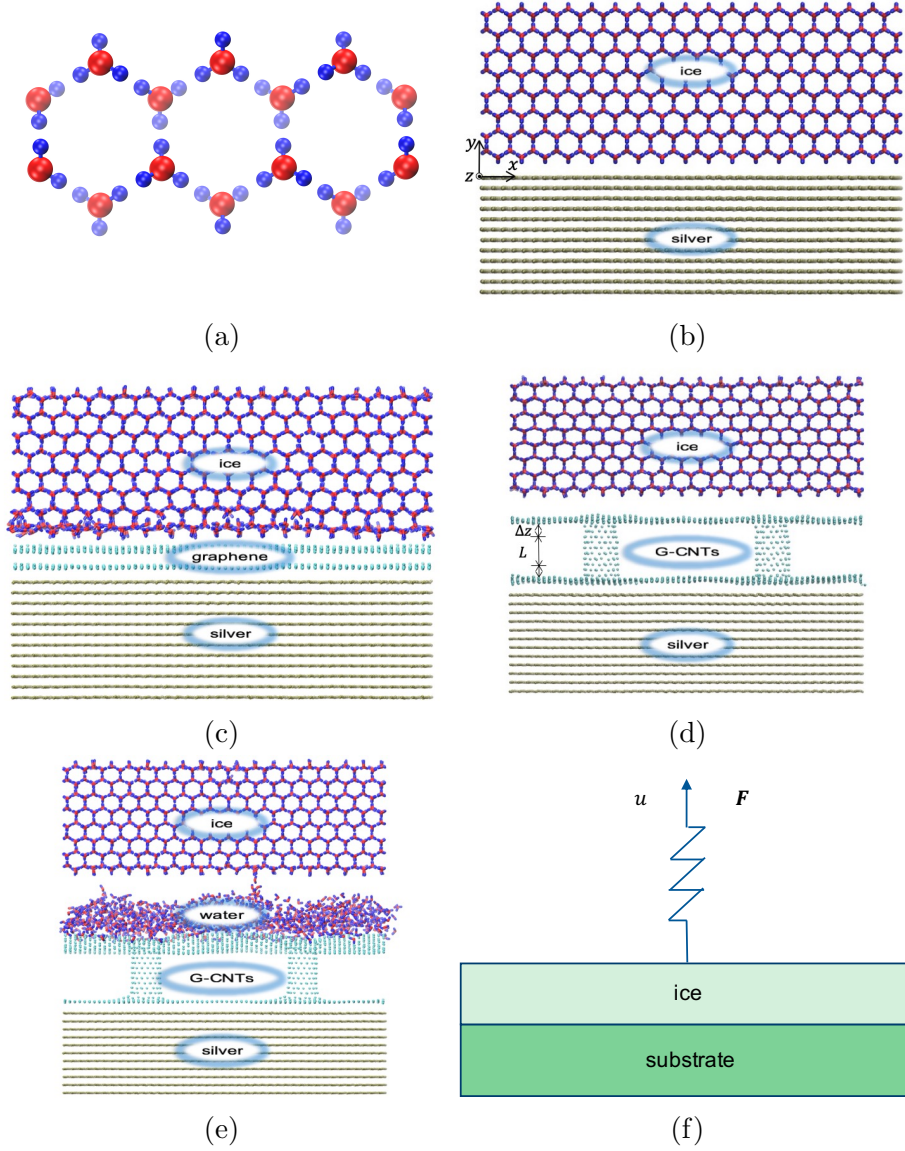


Figure 4.10: Sketch of the MD simulation systems. (a) The model of ice I_h . Simulation systems of (b) ice and silver, (c) multi-layers of graphene coating, (d) G-CNTs coating, (e) water lubricating layer and G-CNTs coating, (f) SMD method setup for probing the adhesion stress between the ice and substrate. The direction of the force detaching ice from the substrate is also illustrated. Three substrates are considered in this work and silver is used as the example in this plot.

4.2.2 MD simulation strategy

The Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package is employed to perform all simulations, and the periodic boundary conditions are used in all three directions. It should be pointed out that a vacuum region with the same thickness from the top of the ice to the bottom of the substrate is added to the top of the ice to eliminate the interaction between the top ice atoms and the bottom substrate atoms resulting from the periodic boundary condition.

The TIP4P/ice model ([Abascal et al., 2005](#)) is used for the ice and water lubrication layer as it has been validated to depict the bulk and near freezing point properties of water and ice reasonably well. For example, the TIP4P/ice model predicts a freezing point of 272.2 K for ice I_h that is reasonably close to the value of 273.15 K observed in the experiment which is compared to other widely used water models such as the SPC/E and TIP4P (the freezing point predicted by these two models is 215 K or 232 K , respectively ([Abascal et al., 2005](#))). The PPPM method is applied to solve long-range electrostatic interactions of ice/water molecules, while the SHAKE algorithm for constraining the bonds and angles is employed to obtain a larger time step of 1 fs in all simulations ([Andersen, 1983](#)). Moreover, all wall substrates which are electrically neutral interact with the ice or water molecules through the Van der Waals force. For the graphene sheet and G-CNTs sandwiched between the ice and silver substrate, the intralayer interactions among carbon atom are simulated with the optimized Tersoff potential ([Lindsay and Broido, 2010](#); [Alexeev et al., 2015](#)), while interlayer carbon atoms interactions are depicted by the Lennard-Jones (LJ)

potential function with parameters ([Girifalco et al., 2000](#)):

$$U(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right], \quad (4.8)$$

where ϵ is the well-depth of the Lennard-Jones potential and σ is the finite distance at which the inter-particle potential is zero. Interactions between silver and silver, copper and copper, silicon and silicon atoms are also described by the LJ potential function, embedded atom method (EAM) and Tersoff potentials, respectively. Moreover, the LJ function is also applied to model the interactions between two different materials. The two parameters in the LJ model are computed from the Lorentz-Bertholot rule ([Lorentz, 1881](#)) except that those are explicitly illustrated in Table 4.3.

Table 4.3: The depth of the potential well ϵ and the size of the particle σ in the Lennard-Jones potential for various atoms.

Material	σ (nm)	ϵ (eV)
Ag-Ag	0.2551	0.4080 (Papanikolaou, 2017)
C-C	0.3276	4.6×10^{-3} (Lindsay et al., 2011)
C-O	0.319	4.908×10^{-3} (Li et al., 2013b)
Cu-O	0.27172	63.87×10^{-3} (Mao and Zhang, 2014)
Cu-C	0.3225	19.996×10^{-3} (Fuentes-Cabrera et al., 2011)
Si-O	0.2633	15.11×10^{-3} (Pham et al., 2013)
Si-C	0.3555	5.955×10^{-3} (Shen et al., 2013)

To clarify the effect of the cut-off distance in the LJ potential, we simulate the ice detaching from the silver substrate with three values of cut-off radii, i.e., 1.0, 2.0 and 3.0 nm, while the adhesion stress and computational cost for each case are shown in Fig. 4.11. One can find that the computational expense increases significantly, where the ice adhesion stress almost maintains a constant value with the increase of the cut-off radius. Therefore, the LJ potential is truncated using a cut-off distance of 1.0 nm for all simulation cases in this work ([Kim and Yethiraj, 2008](#)).

The energy minimization is firstly conducted for simulation systems to

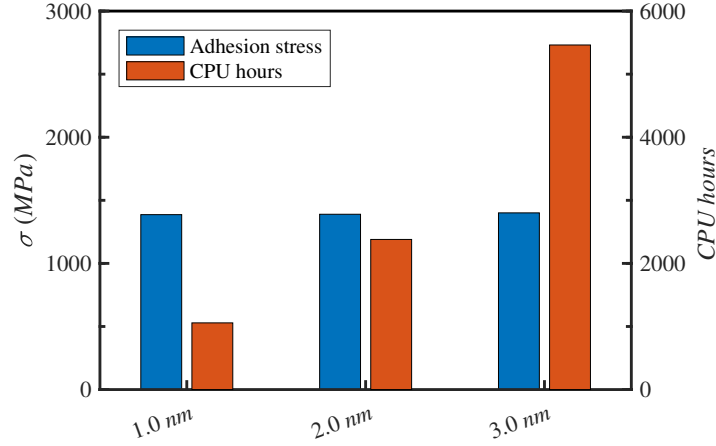


Figure 4.11: Ice adhesion stress and computational time for ice-silver simulation system with various cut-off radii in the LJ potential.

eliminate any possible close contacts among atoms. Then, the ice is let to adhere to the substrate with or without coating through the equilibration process, and the obtained equilibrated structures are applied to examine the ice adhesion stress. All simulations are performed under the NVT ensemble at various temperatures for different models, where the Langevin thermostat method is employed to adjust the temperature to the desired constant value (Schneider and Stoll, 1978b). The temperature of the ice-substrate simulation system with or without coating is maintained at 100 K , while the temperature of the water lubricating layer is kept at 275 K .

4.2.3 Steered molecular dynamics method

The steered molecular dynamics (SMD) (Grubmüller et al., 1996) is a method developed based on MD, and is a powerful tool to investigate the chain dynamics at the interfacial domain. The method has been widely employed to examine the interface characteristics for various systems such as bio-materials (Grubmüller et al., 1996) and polymers (Min et al., 2016),

etc. In this method, a fictitious SMD point connected by a virtual spring to all of the ice atoms is added. The point is displaced with a constant velocity (u), then a force is imposed on the ice to detach the ice from various substrates. The virtual spring force is determined by

$$U = \frac{1}{2}k(ut - (\mathbf{R}(t) - \mathbf{R}_0) \cdot \mathbf{n})^2, \quad (4.9a)$$

$$\mathbf{F} = -\nabla U_s, \quad (4.9b)$$

where $\mathbf{n}$ is an unit vector for the direction of pulling and t is time. $\mathbf{R}(t)$ and $\mathbf{R}_0$ are the current and the initial displacement of the center of mass (COM) of the atoms being pulled (ice in this work), respectively. k is the stiffness coefficient of spring, which is $500 \text{ KJ}/(\text{mol}^{-1}\text{nm}^{-2})$. The constant velocity u for the SMD point is 0.5 nm/ns . U and $\mathbf{F}$ are the potential energy and virtual spring force, respectively. The pulling force $\mathbf{F}$ measured by the distance between the COM of ice and the spring is observed every $1.0 \times 10^{-4} \text{ ns}$, then the ice adhesion stress can be calculated from the following equation:

$$\sigma = \frac{\mathbf{F}_{max}}{A}, \quad (4.10)$$

where $\mathbf{F}_{max}$ is the maximum value of the virtual spring force, and A is the contact area between ice and the substrate. Three independent simulations are conducted for detaching ice from the substrate for all the cases, where the average value is reported in the following.

To validate our simulation, the SMD method is firstly applied to examine the adhesion stress of ice on the atomic smooth surface of a one-layer graphene sheet. The obtained ice adhesion stress is 321.18 MPa , which is in agreement with the value of 364 MPa in reference (Bao et al., 2018). This validates the accuracy of the MD setup in this work.

4.2.4 The base case without coating

The ice adhesion dynamics on our target wall substrate “silver” surface shown in Fig. 4.10b are explored (the detaching process on the copper or silicon surface is similar, and is not shown here for brevity). As shown in Fig. 4.12, the distance between the ice and the silver substrate is arbitrarily set, which converges to a constant value during the process of equilibration simulation, indicating that the ice attaches to the silver substrate stably. Then, a virtual spring placed on the COM of ice moves upward to detach the ice, whose spring force profile is shown in Fig. 4.13a. The force increases gradually, which is followed by a sudden drop to around zero illustrating that the ice is detached from the silver surface completely. Four

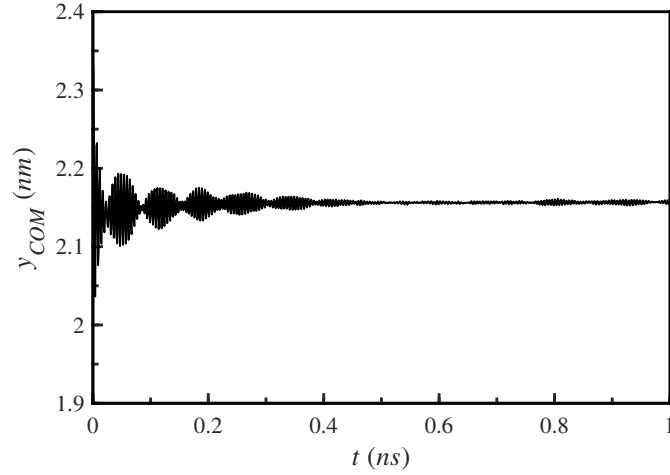
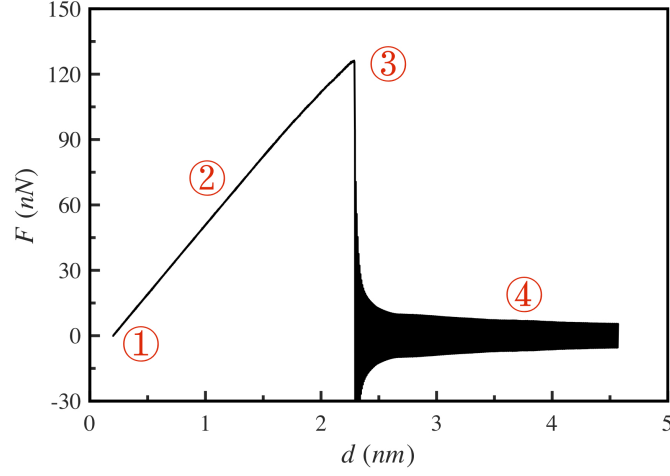


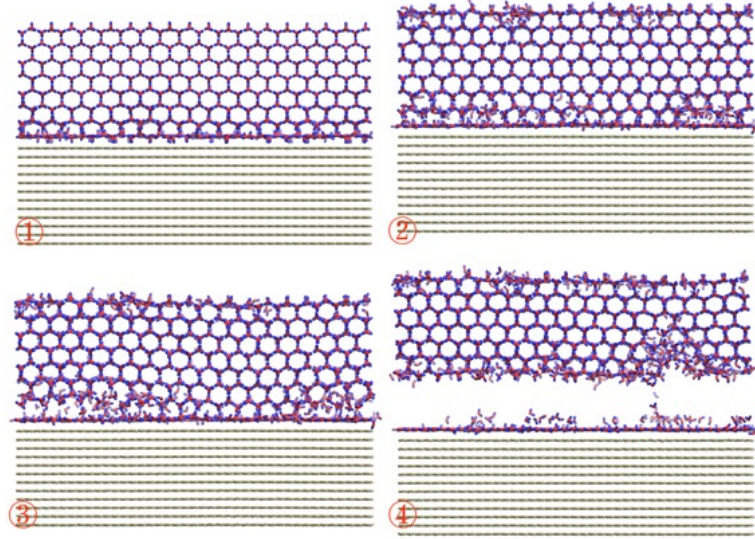
Figure 4.12: The position of center-of-mass of the ice during equilibration simulation process.

labels mark different states of the detaching process, where corresponding snapshots of the simulation system are shown in Fig. 4.13b. The ice is mainly ripped at one side, which is followed by the other side before completely detached from the silver surface. This is because the pulling stress is concentrated on the contact edges of the ice, similarly to the previous experiment (Subramanyam et al., 2013). Finally, substituting the peak value

of the pulling force in Fig. 4.13a into Eq. (4.10), the ice adhesion stress on the silver substrate is obtained as 1386.46 MPa . Similarly, the ice adhesion stresses computed for the copper and silicon surfaces are 1366.33 MPa and 286.18 MPa , respectively.



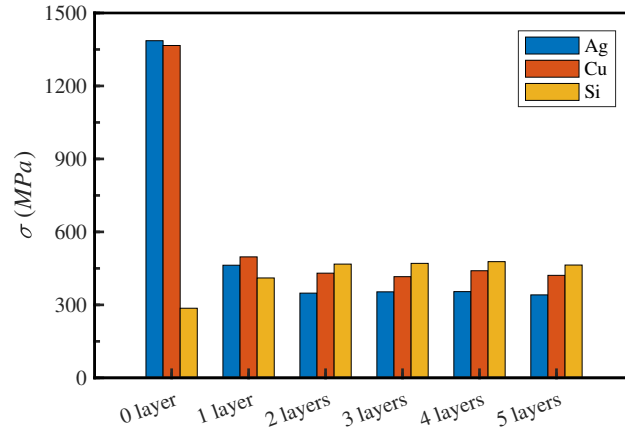
(a)



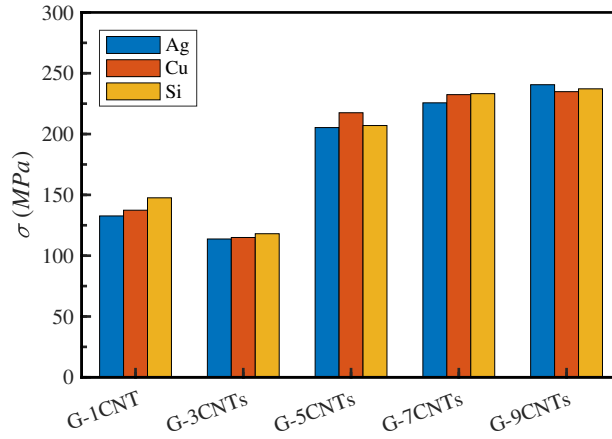
(b)

Figure 4.13: (a) Spring force profile and (b) snapshots of the ice detaching from the silver surface.

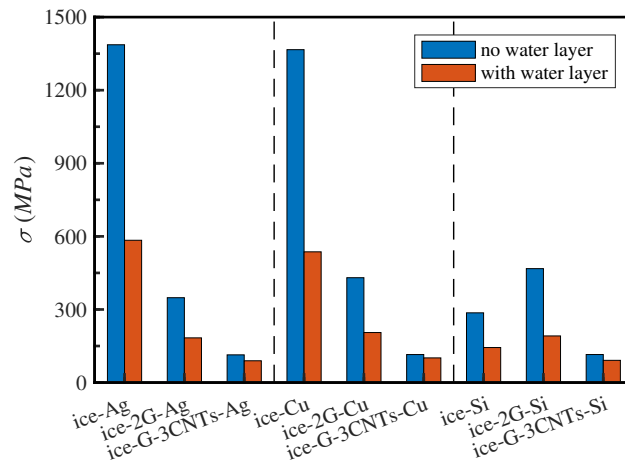
4.2. REDUCTION OF ATOMISTIC ICE TENSILE STRESS BY GRAPHENE-CARBON NANOTUBE COATING



(a)



(b)



(c)

Figure 4.14: Ice adhesion stress at different wall surfaces with (a) graphene sheets, (b) G-CNT coating and (c) water lubricating layers.

4.2.5 Ice adhesion reduction by anti-icing coatings

As aforementioned in Section 4.2, the graphene sheet presents excellent hydrophobicity. Hence, multi-layers of graphene sheet and G-CNTs are placed between the ice and the wall substrate to depress the ice tensile stress, respectively. The effectiveness of the coating is then compared with the water lubricating layer between the ice and substrate widely achieved by the thermal de-icing method to identify an optimal approach for reducing ice adhesion stress.

For the substrate with multi-layers of graphene coating, the corresponding ice adhesion stress is shown in Fig. 4.14a. One can observe that the ice adhesion stress almost converges to a constant value when the number of the graphene sheet is larger than two. Compared with the adhesion stress of ice on the silver or copper surface, a significant reduction of 74.88% or 69.56% of the ice adhesion stress can be achieved by coating the silver or copper substrate with two layers of the graphene sheet, which is caused by the low interfacial energy of the graphene sheet, as introduced in Table 4.3.

Conversely, as can be seen in Fig. 4.14a, the multi-layers of the graphene coating has an adverse effect on reducing the low adhesion stress of ice on the hydrophobic silicon surface because of the hydrophobicity and structure of the silicon substrate. To validate, the energy potential parameter ϵ_{Si-O} is arbitrarily increased to induce different wettability conditions, and the results are summarized in Fig. 4.15. One can observe that the ice adhesion stress reaches to almost a constant value of 1144.45 MPa when the silicon is changed from a hydrophobic to hydrophilic surface. Also, similar to the explanation in the previous study (Ramos-Alvarado et al., 2016a,b), the planar atomic density of the graphene coating is much higher than that of the silicon plane contacting ice, i.e., there are 3588 and 613 atoms for each

graphene sheet and the silicon plane, respectively. Therefore, the interaction force per unit area for the graphene sheet is much larger than that for the low-density silicon surface although the energy potential parameter ϵ_{Si-O} is larger than ϵ_{C-O} , as shown in Table 4.3.

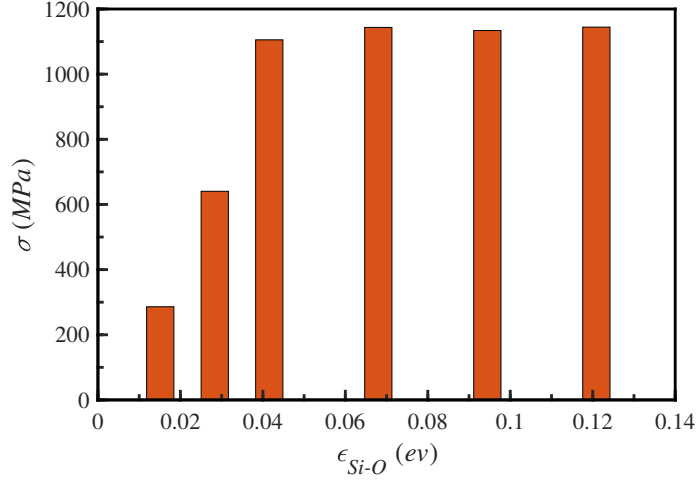


Figure 4.15: Adhesion stress of ice attached on the silicon surface at various interaction parameters. One should note that the maximum ϵ_{Si-O} is computed from the Lorenz-Bertholot rule in Section 4.2.2, and the default ϵ_{Si-O} is 0.01511 *ev* (see Table 4.3) in other simulation cases except in this figure.

In addition, the G-CNTs structure sketched in Fig. 4.10d is placed between the ice and the substrate to analyze the adhesion characteristics. We change the number of carbon nanotubes (CNTs) (i.e., 1, 3, 5, 7 and 9) connecting the two graphene sheets while the length of each CNT is fixed at 1.0 *nm*. The obtained average ice adhesion stress is highlighted in Fig. 4.14b. The ice adhesion stress increases gradually after a slight drop with the increase of the number of CNTs, where the minimum value is observed when the two graphene sheets are connected by three CNTs. The non-monotonic behaviour is influenced by the synergetic effects of rigidity and the number of carbon atoms on the graphene sheet directly contacting with the ice. With the number of carbon nanotubes between the two graphene sheets increas-

ing from 1 to 9, the number of carbon atoms at the top graphene sheet, as sketched by green atoms in Fig. 4.16, reduces from 3560 to 3448, and consequently the adhesion area between ice and the graphene sheet drops. At the same time, the buckling phenomenon of the top graphene, which has a positive effect on reducing the ice adhesion stress to be elaborated on in Section 4.2.6, becomes weaker. Besides, one can observe that the tensile stresses of ice attaching on the silver, copper and silicon substrates with G-CNTs coatings are almost the same. This validates our postulation as mentioned in Section 4.2 that the adhesion force on the ice is mainly contributed by the hydrophobic G-CNTs coating, which is independent on the substrates. Comparing Fig. 4.14b with Fig. 4.14a, the structure of two graphene sheets connected by three carbon nanotubes (G-3CNTs, namely, 3 carbon nanotubes per 0.0335 nm^2) is more effective in depressing the ice adhesion stress than the multi-layers graphene sheet coating, which can reduce the adhesion stress of ice on the silver, copper and silicon surfaces by 91.80%, 91.59% and 58.75%, respectively.

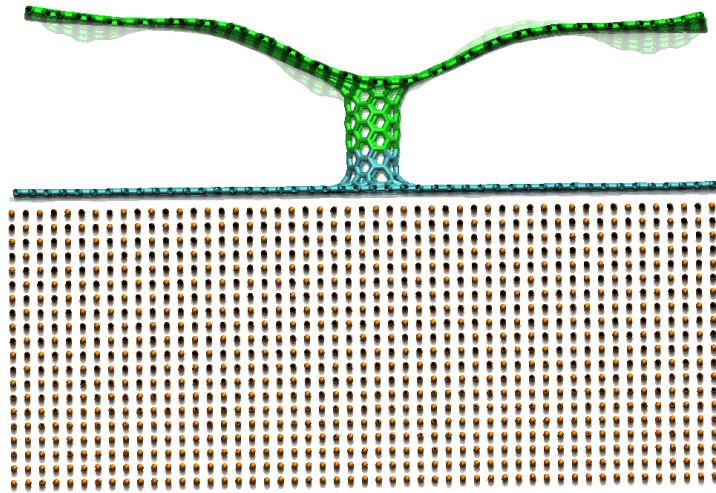
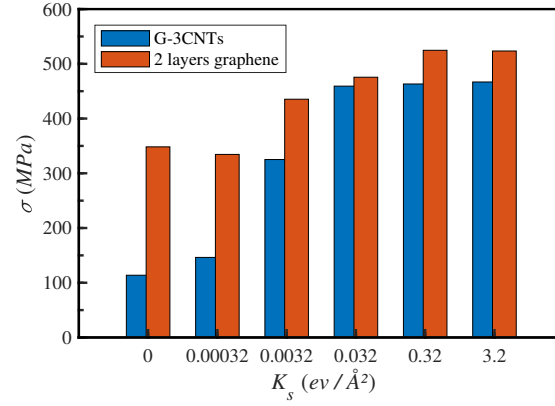


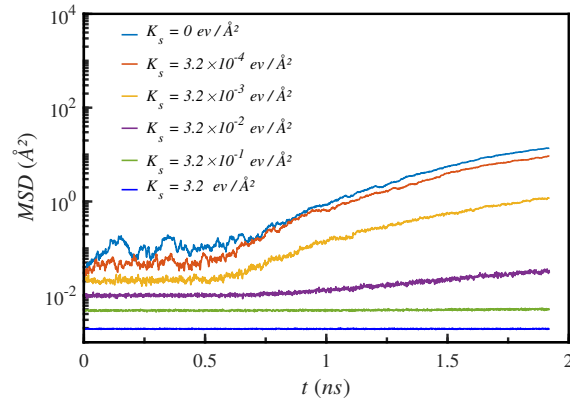
Figure 4.16: The buckling phenomenon of the graphene sheet in G-CNTs coated on the silver surface, the ice structure attached on the top graphene is not shown for brevity.

The ice detaching simulations for systems with the water lubrication layer

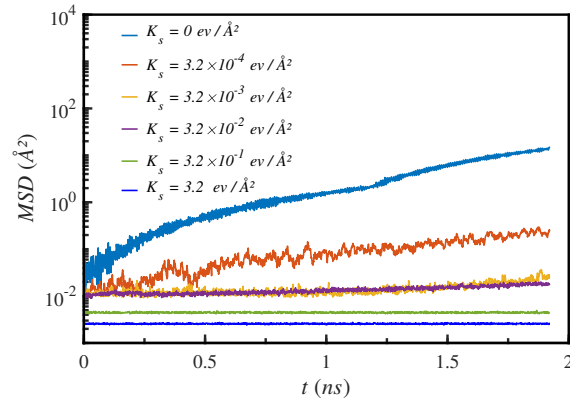
4.2. REDUCTION OF ATOMISTIC ICE TENSILE STRESS BY GRAPHENE-CARBON NANOTUBE COATING



(a)



(b)



(c)

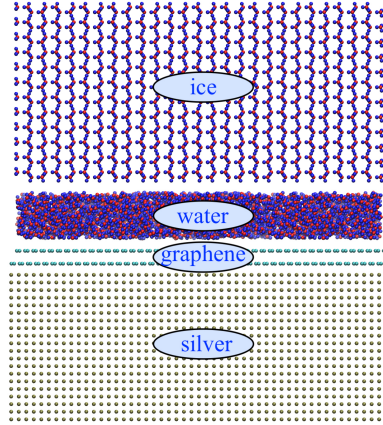
Figure 4.17: The migration dynamics of the ice on the silver substrate and the ice adhesion stress. (a) Effects of the graphene buckling phenomenon on the adhesion stress of ice attached on the silver surface. (b) The mean square displacement of the G-3CNTs. (c) The mean square displacement of the two layers graphene sheet.

are then performed using the same control parameters as introduced in Section 4.2.2. The result indicates that the aqueous layer further reduces the ice adhesion stress, as shown in Fig. 4.14c. Besides, the value of ice adhesion stress for the ice-silver or ice-copper system with an aqueous layer is still larger than that for the ice-2G-silver or ice-2G-copper structure without the lubricating water layer. Meanwhile, the adhesion stress for the ice-G-3CNTs-substrate structure is far less than the ice-substrate with the water lubricating layer. This further confirms that the proposed multi-layers graphene and G-3CNTs coatings have excellent performance on lowering the ice adhesion stress on the silver, copper and all three substrates in this work, respectively. An interesting observation is that the ice and water lubricating layer are detached together from the substrate with or without the graphene sheet or G-CNTs coatings (see Fig. 4.18). This is because the atomistic interactions between the wall surface and the water layer are much weaker than the hydrogen bonds between the water layer and ice.

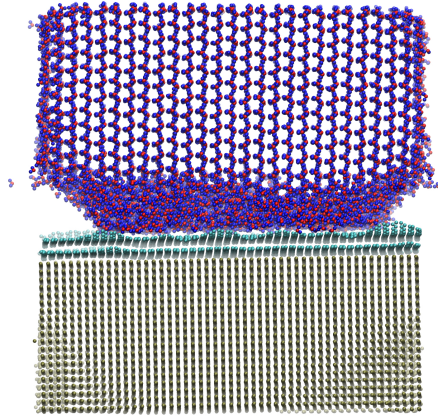
4.2.6 Mechanism of the reduction of ice adhesion stress caused by G-CNTs

The low interfacial energy, that is, the hydrophobicity of the graphene sheet shown in Table 4.3 is a source for reducing ice adhesion stress for the ice-substrate system with multi-layers of graphene sheet or G-CNTs coatings, as illustrated in Section 4.2.4. The buckling phenomenon of the graphene shown in Fig. 4.16 is assumed to be the other reason, and it can be quantified by the mean squared displacement (MSD) defined as

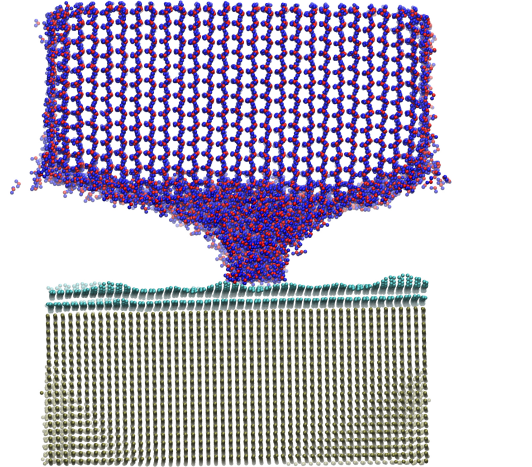
$$MSD(t) = \frac{1}{N} \sum_{i=1}^N |\mathbf{x}^{(i)}(t) - \mathbf{x}^{(i)}(0)|^2, \quad (4.11)$$



(a)



(b)



(c)

Figure 4.18: The process of the ice detached from the silver substrate with two layers of graphene sheet and water lubrication layer. (a) $t = 0 \text{ ns}$. (b) $t = 1.25 \text{ ns}$. (c) $t = 2.50 \text{ ns}$.

where N is the number of particles to be averaged. $\mathbf{x}^{(i)}(t)$ and $\mathbf{x}^{(i)}(0)$ represent the position of the i -th particle at time t and the reference position of the particle, respectively.

To demonstrate the effect of the buckling on the adhesion stress, we add the virtual spring to each carbon atom at the graphene sheets. Then, amplitudes of the carbon atoms and the buckling degree of the graphene can be arbitrarily adjusted by varying the stiffness coefficient of the virtual spring (K_s). Two ice-silver simulation systems sandwiched by the G-3CNTs and the two layers of graphene that show good performance in reducing the ice adhesion stress are chosen, and the ice adhesion stress at various K_s is depicted in Fig. 4.17a. Although each simulation system at a specified K_s has the same energy well depth, a distinct upward trend of the ice adhesion stress is observed at larger K_s where the MSD of the graphene sheet drops as shown in Fig. 4.17b and Fig. 4.17c. This validates our postulation that the buckling phenomenon of the graphene sheet has a positive effect on reducing the ice adhesion stress. Also, the ice adhesion stresses gradually converge for these two simulation systems when $K_s \geq 0.32 \text{ eV}/\text{\AA}^2$ or $MSD \leq 10^{-2} \text{\AA}^2$, suggesting that the ice adhesion stress peaks at a constant value for the absolutely smooth surface.

Furthermore, the ice adhesion stress obtained from MD simulations is larger than the typical experimental value of $\sim 1 \text{ MPa}$. The difference is mainly caused by the large velocity of the virtual spring imposed on the ice in the SMD approach in Section 4.2.3 for the sake of maintaining the computational cost to a reasonable level. It is also worth noting that the ice detaching stress increases logarithmically with the loading rate (Marszalek et al., 1999; Wu et al., 2015). The loading rate does not affect our conclusion that the adhesion stress of ice can be reduced dramatically by coating the silver, copper and silicon with the G-3CNTs structure, as all cases are

examined by using the same loading rate in this work.

4.3 Conclusions

In this chapter, thermal de-icing and icephobic coatings are studied by molecular dynamics simulations. For the thermal de-icing problem on a flat wall, we explore the effects of the thickness of ice layer H , wall temperature T_w and wettability on the melting time and the energy consumption. Meanwhile, two icephobic coating structures including the multi-layers graphene sheet and graphene and carbon nanotubes junctions (G-CNTs) are proposed for the first time, the steered molecular dynamics approach is then employed to compute the ice adhesion stress.

Compared with previous studies, we revealed for the first time that the ice accumulated on a hydrophobic surface requires more time to melt compared with the hydrophilic wall, whilst the energy cost during the thermal de-icing process is independent of the wettability of the wall surface. Also, the melting time can be approximated as $t(T_w, H) = (9.033H - 7.903)/(T_w - 273.15) + 0.1158H - 0.4005$, illustrating a linear function with respect to H and $1/(T_w - 273.15)$. The energy cost can be modelled as a linear function of the wall temperature with the slope increasing as the ice thickness: $E(T_w, H) = (2.5H + 2.078)T_w - 538.6H - 543$.

The ice adhesion stresses for various simulation systems with/without various coatings satisfy: ice-Ag (ice-Cu) > ice-water-Ag (ice-water-Cu) > ice-2G-Ag (ice-2G-Cu) > ice-water-2G-Ag (ice-water-2G-Cu) > ice-G-3CNTs-Ag (ice-G-3CNTs-Cu) > ice-water-G-3CNTs-Ag (ice-water-G-3CNTs-Cu), and ice-2G-Si > ice-Si > ice-water-2G-Si > ice-water-Si > ice-G-3CNTs-Si > ice-water-G-3CNTs-Si. Namely, the aqueous layer between the ice and

the hydrophobic/hydrophilic wall has a positive effect on lowering ice adhesion stress. Two layers of the graphene sheet coating can reduce the tensile stress of ice accumulating to the hydrophilic silver/copper surface due to the hydrophobicity of the coating. Although graphene is more hydrophobic than silicon, however, the coating has an adverse effect on lowering the ice tensile stress on the silicon surface. This is because the planar atomic density of the graphene coating is much higher than that of the silicon plane contacting ice, and then the interaction force per unit area for the graphene sheet is much larger than that for the low-density silicon surface. Also, a noticeable reduction of the ice tensile stress can be achieved by the G-3CNTs structure coated on the hydrophobic/hydrophilic wall surface. This work provides the insight of the physical process of thermal de-icing and guidance to the design of de-icing systems for aircraft, roads, etc. Two novel methods for lowering ice adhesion are proposed, and they can guide the design of icephobic wall surfaces in general.

Chapter 5

Conclusions and future work

5.1 Summary of current work

In this thesis, the heat transfer and resistance characteristics of fluids in micro- and nano-scale are investigated by applying the analytical solution and numerical modelling techniques including computational fluid dynamics (CFD) and molecular dynamics (MD) simulation.

For Macroscale flow and heat transfer featuring no-slip boundary condition and neglecting viscous dissipation, the fully developed temperature is equal to the constant wall temperature based on our analytical solution of the 2D energy equation. However, the fully developed bulk temperature of fluid converges to a constant value which is higher than the constant wall temperature regardless of the inflow temperature condition (i.e., $T_{fluid} \geq T_{wall}$ or $T_{fluid} < T_{wall}$) due to that the viscous dissipation becomes dominant in micro- and nano-scale heat transfer. The value of the temperature overshoot increases linearly with the Brinkman number, drops slightly at higher the Knudsen number, and is almost independent of the Péclet number. It is

worth noting that if fluid is used to cool the wall with uniform temperature, there is a critical point where the fluid bulk temperature reaches the same value as wall temperature and the Nusselt number becomes ill-defined at this point. This point moves much closer to the micro-scale channel entrance at increasing the Brinkman and Péclet numbers. Conversely, at a larger Knudsen number, the point moves towards the end of the channel.

Besides, the resistance coefficient as an important factor of fluid flow is generally computed from the Bernoulli's equation. However, this method cannot visualize the flow resistance loss at every point in the flow field. Therefore, a new approach, second law analysis (SLA) based on the local entropy generation rate is proposed to compute and visualize the flow resistance of fluid with uniform temperature. This novel approach is validated by comparing the obtained resistance coefficients for laminar pipe, channel with/without a sudden contraction component (SCC) flow with those values computed from the traditional Bernoulli's equation. According to the SLA approach, the flow resistance of fluids results from two factors: wall drag force work (equal to 0 for no-slip flow) and viscous dissipation in the flow field related to the local entropy generation rate. Also, the existence of the velocity slip phenomenon is in favor of the reduction of flow resistance of pipe/channel flow. However, at $Re \leq 10$, the flow resistance coefficient for the SCC, denoted as K_{SCC} , increases monotonously with L_{slip}^* and $1/Re$ and nonlinearly with R_{area} , and at $R_{area} \geq 8$, the resistance coefficient can be modelled as $K_{SCC} = (0.4454L_{slip}^{*3} - 1.894L_{slip}^{*2} + 2.917L_{slip}^* + 8.909)/Re$.

Then, MD simulations are conducted to study novel features (i.e., velocity slip, temperature jump, density layering and non-uniform viscosity profile) that have significant effects on the micro- and nano-scale flow and heat transfer. A dramatic reduction of the velocity slip length is observed when moving from hydrophobic to hydrophilic surfaces. The thermal slip length

is noticeably affected by the liquid argon atoms layering in the proximity of the wall and more specifically by the first peak value of argon atoms adjacent to the fluid-wall interface. Hence, the thermal slip length can be tuned via varying the wall wettability to change the first density peak value.

Besides, to explore novel and efficient ice removal techniques, the thermal de-icing and coatings are studied as examples of the active and passive de-icing methods, respectively. MD simulations are then performed to understand the dynamic mechanism from the molecular level. When the thermal de-icing method (i.e., heating the wall to melt ice) is applied to remove the ice accumulated on the wall surface, the melting time is almost bilinear with respect to the ice thickness and the reciprocal of the wall temperature, and converges to a constant value when the wall temperature is higher than 313.15 K . The energy cost during the thermal de-icing process can be modelled as a linear function of the wall temperature with the slope increasing as the ice thickness. Compared with a hydrophilic wall, more time and almost constant energy are required to melt the ice accumulated on a hydrophobic surface which is generally considered as the icephobic material and prevents ice accretion.

In addition, a novel structure, the graphene and carbon nanotubes junction (G-CNTs), is proposed as an icephobic coating. The ice adhesion stresses on the silver, copper and silicon substrates can be significantly reduced by 91.80%, 91.59% and 58.75% through coating these wall surfaces with the G-CNTs structure. This observation sheds light on the design of the icephobic wall surface and the development of de-icing techniques.

5.2 Future work

Based on this thesis, the future work is summarised in the following:

1. Development of a continuum and molecular dynamics hybrid algorithm for micro- and nano-scale flow.

For the first-order velocity slip and temperature jump wall boundary conditions applied in obtaining the analytical solution of the continuum-based 2D energy equation, two parameters including tangential momentum coefficient and thermal accommodation coefficient are commonly assumed to be constant values. These two parameters have strong effects on the velocity slip length and the Kapitza thermal resistance. However, they strongly depend on the materials of fluids and the wall, local pressure, velocity and the mean direction of the local flow. Besides, a series of distinct molecular layers form the density layering in the vicinity of the fluid-wall interface and produce the non-uniform density and viscosity profiles. Although molecular dynamics simulation can capture these features of the fluid-wall interface, it is unrealistic to apply full MD simulations to investigate flow and heat transfer at micro- and nano-scale due to the limitations of computational time and memory. Therefore, it is desirable to design the hybrid modelling approach combining continuum fluid dynamics and molecular dynamics, and the flow and heat transfer at the interface and the bulk region are respectively described by the continuum-based governing equations and the atomistic method.

2. Exploration of the physics of ice melting

Although the melting time and energy consumption of thermal de-icing are well clarified in Section 4.1 by conducting molecular dynam-

ics simulations, the fundamental mechanisms during the ice melting, i.e., defects of the hydrogen bond network, are now well understood. Also, a tetrahedral entropy per molecule defined by Kumar et al. (Kumar et al., 2009) was found to be strongly related to the number of hydrogen bonds of ice/water molecules (Guardia et al., 2015), and we will analyze the observed melting process from the view of the entropy in our future work.

In addition, a quasi-liquid layer (QLL) between the ice and solid wall has been widely reported when the temperature of ice is below its bulk melting point, and the physical mechanism for this phenomenon is not well clarified. Hence, more efforts should be focused on these interesting issues.

3. Simulations of ice crystallisation

Although we can apply the thermal de-icing method reported in Section 4.1 to remove ice that has been accumulated on the solid surface, another important measure is to take measures to impede the formation of ice. For example, antifreeze protein can bind to the wall surface to inhibit the growth of the ice crystal. However, the binding mechanism, that is, how the antifreeze protein recognizes and attaches itself to ice, is an unsolved fundamental question. Therefore, a future line of work is to apply molecular dynamics as an ideal method to explore the binding mechanism.

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Appendices

Appendix A

Least-square method to compute coefficients

According to boundary conditions, we have

$$\sum_{n=1}^{\infty} A_n f_n(\eta) = 1 - \theta_1(\eta) . \quad (\text{A.1})$$

After choosing some discrete points $(\eta_0, \eta_1, \dots, \eta_p)$ in y direction and substituting these points in Eq. (A.1), we can obtain

$$\begin{aligned} A_1 f_1(\eta_0) + A_2 f_2(\eta_0) + \dots + A_N f_N(\eta_0) &= 1 - \theta_1(\eta_0) , \\ A_1 f_1(\eta_1) + A_2 f_2(\eta_1) + \dots + A_N f_N(\eta_1) &= 1 - \theta_1(\eta_1) , \\ &\vdots \\ A_1 f_1(\eta_p) + A_2 f_2(\eta_p) + \dots + A_N f_N(\eta_p) &= 1 - \theta_1(\eta_p) . \end{aligned} \quad (\text{A.2})$$

Rewriting Eq. (A.2) into a matrix form

$$\begin{bmatrix} f_1(\eta_0) & f_2(\eta_0) & \cdots & f_N(\eta_0) \\ f_1(\eta_1) & f_2(\eta_1) & \cdots & f_N(\eta_1) \\ \vdots & \vdots & \vdots & \vdots \\ f_1(\eta_p) & f_2(\eta_p) & \cdots & f_N(\eta_p) \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \\ \vdots \\ A_N \end{bmatrix} = \begin{bmatrix} 1 - \theta_1(\eta_0) \\ 1 - \theta_1(\eta_1) \\ \vdots \\ 1 - \theta_1(\eta_p) \end{bmatrix}. \quad (\text{A.3})$$

The coefficients A_n can be calculated as

$$\begin{bmatrix} A_1 \\ A_2 \\ \vdots \\ A_N \end{bmatrix} = \begin{bmatrix} f_1(\eta_0) & f_2(\eta_0) & \cdots & f_N(\eta_0) \\ f_1(\eta_1) & f_2(\eta_1) & \cdots & f_N(\eta_1) \\ \vdots & \vdots & \vdots & \vdots \\ f_1(\eta_p) & f_2(\eta_p) & \cdots & f_N(\eta_p) \end{bmatrix}^{-1} \begin{bmatrix} 1 - \theta_1(\eta_0) \\ 1 - \theta_1(\eta_1) \\ \vdots \\ 1 - \theta_1(\eta_p) \end{bmatrix}. \quad (\text{A.4})$$

Appendix B

Development of the semi-implicit scheme B

The linear Navier slip model can be rewritten as based on aforementioned analyses in Eq. (2.51) and Eq. (2.52)

$$\mathbf{U}_{wt} = C_2 \mathbf{U}_{Ct} = C_2 (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \bullet \mathbf{U}_C , \quad (\text{B.1})$$

where C_2 is a function of velocity slip length L_{slip} . Eq. (B.1) can be further rewritten as

$$\mathbf{U}_{wt} = C_2 \begin{bmatrix} 1 - n_x^2 & -n_x n_y & -n_x n_z \\ -n_x n_y & 1 - n_y^2 & -n_y n_z \\ -n_x n_z & -n_y n_z & 1 - n_z^2 \end{bmatrix} \cdot \begin{bmatrix} U_{Cx} \\ U_{Cy} \\ U_{Cz} \end{bmatrix} . \quad (\text{B.2})$$

After reformulating Eq. (B.2), we have

$$\begin{bmatrix} U_{wt,x} \\ U_{wt,y} \\ U_{wt,z} \end{bmatrix} = C_2 \begin{bmatrix} 1 - n_x^2 & 0 & 0 \\ 0 & 1 - n_y^2 & 0 \\ 0 & 0 & 1 - n_z^2 \end{bmatrix} \cdot \begin{bmatrix} U_{Cx} \\ U_{Cy} \\ U_{Cz} \end{bmatrix} + C_2 \begin{bmatrix} 0 & -n_x n_y & -n_x n_z \\ -n_x n_y & 0 & -n_y n_z \\ -n_x n_z & -n_y n_z & 0 \end{bmatrix} \cdot \begin{bmatrix} U_{Cx} \\ U_{Cy} \\ U_{Cz} \end{bmatrix}. \quad (\text{B.3})$$

At time step i and $i - 1$, $\mathbf{U}_{wt}$ can be represented as

$$\begin{bmatrix} U_{wt,x}^i \\ U_{wt,y}^i \\ U_{wt,z}^i \end{bmatrix} = \begin{bmatrix} C_2 (1 - n_x^2) \\ C_2 (1 - n_y^2) \\ C_2 (1 - n_z^2) \end{bmatrix} \cdot \begin{bmatrix} U_{Cx}^i \\ U_{Cy}^i \\ U_{Cz}^i \end{bmatrix}^T + \begin{bmatrix} C_2 (-n_x n_y U_{Cy}^i - n_x n_z U_{Cz}^i) \\ C_2 (-n_x n_y U_{Cx}^i - n_y n_z U_{Cz}^i) \\ C_2 (-n_x n_z U_{Cx}^i - n_y n_z U_{Cy}^i) \end{bmatrix}. \quad (\text{B.4})$$

and

$$\begin{bmatrix} U_{wt,x}^{i-1} \\ U_{wt,y}^{i-1} \\ U_{wt,z}^{i-1} \end{bmatrix} = \begin{bmatrix} C_2 (1 - n_x^2) \\ C_2 (1 - n_y^2) \\ C_2 (1 - n_z^2) \end{bmatrix} \cdot \begin{bmatrix} U_{Cx}^{i-1} \\ U_{Cy}^{i-1} \\ U_{Cz}^{i-1} \end{bmatrix}^T + \begin{bmatrix} C_2 (-n_x n_y U_{Cy}^{i-1} - n_x n_z U_{Cz}^{i-1}) \\ C_2 (-n_x n_y U_{Cx}^{i-1} - n_y n_z U_{Cz}^{i-1}) \\ C_2 (-n_x n_z U_{Cx}^{i-1} - n_y n_z U_{Cy}^{i-1}) \end{bmatrix}. \quad (\text{B.5})$$

At time step i , we note that the first term of the right side of the equation is the function of the velocity component of mesh cell central point in x direction. However, the second term is related to mesh cell's velocity in the other two directions. Hence, we can perform the linearization of this

boundary condition as follows:

$$\begin{aligned}
& \begin{bmatrix} C_2 (-n_x n_y U_{Cy}^i - n_x n_z U_{Cz}^i) \\ C_2 (-n_x n_y U_{Cx}^i - n_y n_z U_{Cz}^i) \\ C_2 (-n_x n_z U_{Cx}^i - n_y n_z U_{Cy}^i) \end{bmatrix} \\
& \approx \begin{bmatrix} C_2 (-n_x n_y U_{Cy}^{i-1} - n_x n_z U_{Cz}^{i-1}) \\ C_2 (-n_x n_y U_{Cx}^{i-1} - n_y n_z U_{Cz}^{i-1}) \\ C_2 (-n_x n_z U_{Cx}^{i-1} - n_y n_z U_{Cy}^{i-1}) \end{bmatrix} \\
& = \begin{bmatrix} U_{wt,x}^{i-1} \\ U_{wt,y}^{i-1} \\ U_{wt,z}^{i-1} \end{bmatrix} - \begin{bmatrix} C_2 (1 - n_x^2) \\ C_2 (1 - n_y^2) \\ C_2 (1 - n_z^2) \end{bmatrix} \cdot \begin{bmatrix} U_{Cx}^{i-1} \\ U_{Cy}^{i-1} \\ U_{Cz}^{i-1} \end{bmatrix}^T.
\end{aligned} \tag{B.6}$$

Now, the velocity slip model can be obtained for time step i

$$\begin{aligned}
\begin{bmatrix} U_{wt,x}^i \\ U_{wt,y}^i \\ U_{wt,z}^i \end{bmatrix} &= \begin{bmatrix} C_2 (1 - n_x^2) \\ C_2 (1 - n_y^2) \\ C_2 (1 - n_z^2) \end{bmatrix} \cdot \begin{bmatrix} U_{Cx}^i \\ U_{Cy}^i \\ U_{Cz}^i \end{bmatrix}^T + \left\{ \begin{bmatrix} U_{wt,x}^{i-1} \\ U_{wt,y}^{i-1} \\ U_{wt,z}^{i-1} \end{bmatrix} \right. \\
&\quad \left. - \begin{bmatrix} C_2 (1 - n_x^2) \\ C_2 (1 - n_y^2) \\ C_2 (1 - n_z^2) \end{bmatrix} \cdot \begin{bmatrix} U_{Cx}^{i-1} \\ U_{Cy}^{i-1} \\ U_{Cz}^{i-1} \end{bmatrix}^T \right\}.
\end{aligned} \tag{B.7}$$

One can note that the second term of the right side of the equal symbol of the above equation is a known value. Then, that equation can be further rewritten as

$$\mathbf{U}_{wt}^i = \begin{bmatrix} C_2 (1 - n_x^2) \\ C_2 (1 - n_y^2) \\ C_2 (1 - n_z^2) \end{bmatrix} \cdot \mathbf{U}_C^i + \left\{ \mathbf{U}_{wt}^{i-1} - \begin{bmatrix} C_2 (1 - n_x^2) \\ C_2 (1 - n_y^2) \\ C_2 (1 - n_z^2) \end{bmatrix} \cdot \mathbf{U}_C^{i-1} \right\}. \tag{B.8}$$

We note that coefficient is

$$\begin{aligned} \begin{bmatrix} C_2 (1 - n_x^2) \\ C_2 (1 - n_y^2) \\ C_2 (1 - n_z^2) \end{bmatrix} &= \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} - \left[(1 - C_2) \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} + C_2 \begin{pmatrix} n_x^2 \\ n_y^2 \\ n_z^2 \end{pmatrix} \right] \\ &= C_1. \end{aligned} \tag{B.9}$$

Hence, Eq. (B.8) can be rearranged as (this equation is also shown in Eq. (2.53c))

$$\mathbf{U}_{wt}^i = C_1 \mathbf{U}_C^i + (\mathbf{U}_{ws}^{i-1} - C_1 \mathbf{U}_C^{i-1}) . \tag{B.10}$$

Appendix C

Resistance coefficient calculated from second law analysis (SLA) for pipe flow

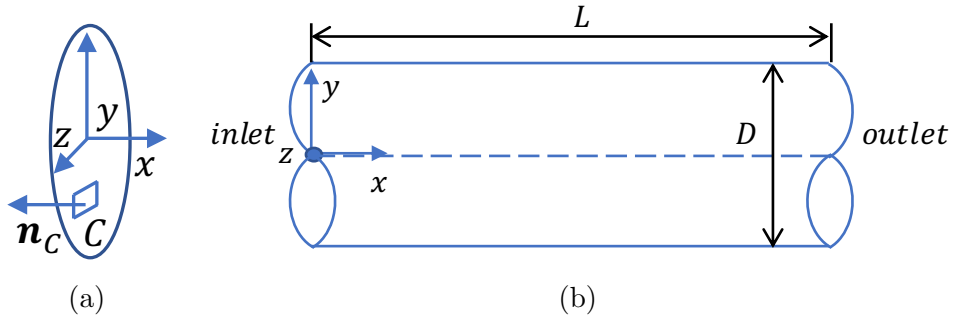


Figure C.1: Sketches of a circular pipe and its inlet. (a) Pipe inlet. (b) Pipe.

When fully developed Poiseuille flow in a horizontal straight pipe is considered, the local entropy generation rate in the cylinder coordinate system becomes

$$\dot{S}_{irr,D}''' = \frac{1}{T} \mu \left(\frac{\partial U_x}{\partial r} \right)^2. \quad (\text{C.1})$$

Substituting the velocity profile, $U_x = \frac{1}{4\mu} \left(-\frac{dp}{dx} \right) (R^2 + 2L_{slip}R - r^2)$, into

Eq. (C.1), the local entropy production rate for Poiseuille flow in horizontal straight circular pipes with linear SBC is

$$\dot{S}_{irr,D}''' = \frac{\mu}{T} \left[\frac{1}{4\mu} \left(-\frac{dp}{dx} \right) (-2r) \right]^2 = \frac{1}{T} \frac{1}{4\mu} \left(-\frac{dp}{dx} \right)^2 r^2. \quad (C.2)$$

Considering the relationship between average velocity and pressure gradient, $U_{ave} = \frac{\int_0^R U_x \cdot 2\pi r dr}{\int_0^R 2\pi r dr} = \frac{1}{8\mu} \left(-\frac{dp}{dx} \right) (R^2 + 4L_{slip}R)$, Eq. (C.2) can be further rewritten as

$$\dot{S}_{irr,D}''' = 16 \frac{\mu}{T} \frac{r^2}{(R^2 + 4L_{slip}R)^2} U_{ave}^2. \quad (C.3)$$

The overall entropy production rate can be determined from

$$\begin{aligned} \dot{S}_{irr,D} &= \int_V \dot{S}_{irr,D}''' dV \\ &= L \cdot \int_0^R 16 \frac{\mu}{T} \frac{r^2}{(R^2 + 4L_{slip}R)^2} U_{ave}^2 \cdot 2\pi r dr \\ &= 8 \frac{\mu\pi L}{T} \frac{1}{\left(1 + 4\frac{L_{slip}}{R}\right)^2} U_{ave}^2. \end{aligned} \quad (C.4)$$

The tangential wall stress vector can be determined when substituting the velocity profile into Eq. (2.51)

$$\boldsymbol{\tau}_{wt} = \mu \left. \frac{\partial \mathbf{U}}{\partial r} \right|_{r=R} = \frac{-R}{2} \left(\frac{-dp}{dx} \right), \quad (C.5)$$

and velocity of fluid in the vicinity of wall can be calculated as when $r = R$

$$\mathbf{U}_{wt} = \frac{L_{slip}R}{2\mu} \left(\frac{-dp}{dx} \right). \quad (C.6)$$

The work of drag force can be denoted after substituting Eq. (C.5) and

Eq. (C.6) into Eq. (2.62) and considering $-\frac{dp}{dx} = \frac{8\mu U_{ave}}{R^2 + 4L_{slip}R}$

$$\begin{aligned} W_{drag} &= - \left[\frac{-R}{2} \left(\frac{-dp}{dx} \right) \cdot \frac{L_{slip}R}{2\mu} \left(\frac{-dp}{dx} \right) \right] \cdot (2\pi R \cdot L) \\ &= \frac{32\pi\mu U_{ave}^2 L R^3 L_{slip}}{(R^2 + 4L_{slip}R)^2} \end{aligned} \quad (C.7)$$

Then, the head loss coefficient can be obtained after substituting Eq. (C.4) and Eq. (C.7) into Eq. (2.61)

$$K = \frac{64}{Re} \frac{1}{1 + 8\frac{L_{slip}}{D}} \frac{L}{D} . \quad (C.8)$$