



Regulation of anti-Fourier heat transfer for non-equilibrium gas flows through micro/nanochannels



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ARTICLE INFO

Article history:

Received 6 October 2016
Received in revised form
6 April 2017
Accepted 6 April 2017

Keywords:

Reduced wall heat flux
Anti-Fourier heat transfer
Shear stress
Cold-to-Hot heat transfer
Rarefied gas flow
DSMC

ABSTRACT

In this study we use the direct simulation Monte Carlo (DSMC) to elaborate on the heat transfer patterns in the pressure-driven rarefied flow through micro/nanochannels. Finite length planar micro/nanochannels are considered using with symmetrical wall heat flux boundary conditions, and the gas flow is considered to be in slip and transition regimes. When considering zero-conductive or cooled walls, the DSMC solution predicts a possibility of the anti-Fourier heat transfer, i.e., the transfer of heat from cold-to-hot regions of the flow field. It turns out that the competition between the contributions of temperature gradient and pressure gradient (shear stress) in the heat flux results in three different heat transfer regimes. The regimes consist of complete hot-to-cold heat transfer regime, the entire anti-Fourier regime, and localized anti-Fourier regime. While the heat flux due to the shear stress is directed from the outlet towards the inlet, the Fourier term is strongly influenced by viscous slip heating, which then acts as a heat source, and contributes to patterns of heat flux on the fluid layer adjacent to the walls. Furthermore, the heat flux regimes for complete or localized cold-to-hot transfer are classified according to the magnitude of the normalized heat flux and the Knudsen number. Additionally, effects of heat flux condition on the mass flow rate are discussed.

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1. Introduction

Current researches involving typical micro/nano-electro-Mechanical-systems (MEMS/NEMS) include investigations of the use of micro/nanosystems for cooling applications. The ability to perform a number of operations on a small unit using miniaturized devices, also known as a Lab-on-a-Chip (LOC) or microfluidics devices, has numerous benefits. However, perfect designs and experimental analysis of such miniature-scale systems are particularly stimulating. In fact, in proportion to their size, the level of thermal power dissipated by electronic components is almost significant, i.e., the power density is substantial. Consequently, these devices require a heat exchanger in micro or nanoscale which is usually in the form of an array of micro or nano-channels. Accordingly, accurate modeling of heat transfer behavior is crucial for these systems. In such systems, the molecular mean free path is not negligible compared to the representative lengths. It is well accepted that the classical equations of hydrodynamics, the Navier-

Stokes and Fourier laws, fail to adequately describe the flow and heat transfer behaviors in micro/nano systems. Therefore, they must be considered as rarefied gas flows, and the flow and heat transfer behaviors shall be described based on kinetic theory. The rarefaction of gas is quantified by the Knudsen number (Kn) as follows.

$$Kn = \lambda/H \quad (1)$$

where λ and H are the gas mean free path and the characteristic dimension of the geometry, respectively. The Knudsen number expresses the ratio of intermolecular collisions to gas-solid collisions. As the classical hydrodynamic equations, including the Navier-Stokes and Fourier laws, are unable to model the rarefaction effects at the transition regime, $Kn > 0.1$, the Boltzmann equation can serve to simulate rarefied gas flows appropriately in microscopic detail [1–4]. Rarefied flow behavior can be detected by careful analysis of the Boltzmann equation, with either deterministic numerical treatment or statistical molecular simulations. Among various molecular-based schemes, direct simulation Monte Carlo (DSMC) is an efficient particle-based scheme uses the probabilistic Monte Carlo technique to solve the Boltzmann equation

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Nomenclature

E_{kin}	Kinetic energy
F_{num}	Real to simulated particle ratio
Kn	Knudsen number
H	Channel height (m)
q	Conductive Heat flux (W/m ²)
q_{vsh}	Viscous slip heating heat flux
Q	Dimensional heat flux
k	Boltzmann constant
d	Molecule diameter (m)
M	Molecular weight (kg/mole)
N_{CM}	Number of incident molecules
T	Temperature (K)
L	Channel length (m)
AR	Channel aspect ratio (L/H)
u	Flow velocity (m/s)
C_p	Specific heat capacity (J/kg.k)
\dot{m}	Mass flow rate (kg/s)
c	Particle velocity (m/s)
n	Number density
P	gas pressure (N/m ²)
Ma	Mach Number
R_f	Random number
S_{kin}	Molecular velocity direction ratio

V_{slip} Slip Velocity

Greek letters

Δs	Surface Area
ΔT_w	Wall temperature correction
λ	Mean free path
ρ	mass density (kg/m ³)
ϵ_{int}	Internal energy of particle
τ	Shear stress (N/m ²)

Subscripts

x	X direction along the channel
w	Channel wall
Y	Y direction across the channel
$avg.$	Average
$char$	Characteristics
des	Design/specified
o	Stream mean parameter
In	Inlet condition
Out	Outlet condition

Superscripts

*	Dimensionless parameters
'	Peculiar velocity component

over a broad range of the Knudsen number.

Some researchers have observed interesting phenomena in micro-nano geometries that do not occur in the continuum regime, i.e. $Kn < 0.001$ [5–26]. For example, the mass flux in channel flow as a function of the Knudsen number reveals a minimum around the unity Knudsen number, the so-called Knudsen paradox phenomenon [5,10,16,19,20,22,25]. A heat flux driven by the velocity gradient is another interesting phenomenon in the rarefied flow [6,11,12,15,17,18], while heat flux is only driven by the temperature gradient in the continuum threshold. Inverse Magnus effect [23] and flow induced by temperature field [21,26] are other unique features reported at rarefied flows regimes. A comprehensive review on the application of moment methods in treating rarefied microflows is reported in Ref. [27].

The anti-Fourier heat transfer is already reported in rarefied flows in the cavity and channel geometries [11,12,14,15,17,18], i.e., the existence of cold-to-hot heat transfer process is demonstrated in the cooling wall cases in the channel flow [15]. However, our literature survey indicates that the details of various patterns of heat transfer of the rarefied flow through micro/nano-geometries were not considered in previous studies. In particular, the counter gradient, anti-Fourier heat transfer in pressure-driven micro/nanoscales channels through a wide range of Knudsen number, the underlying causes behind this behavior, and regulation of different heat transfer regimes were not reported in the literature. Therefore, in this work, a description of simulated flow fields follows for a broad range of test conditions to describe the non-intuitive behavior of heat flow patterns observed in the slip and transition regimes in micro and nanoscale channels. The zero-conductive and the cooling wall boundary conditions are considered in this study, where there is a possibility of anti-Fourier heat transfer. A distinction is made between the contribution of the boundary terms such as viscous slip heating, which exists even in zero-conductive wall conditions and contribute in heat flux bifurcation, and bulk terms such as pressure gradient, which contribute in the constitutive law of the heat flux. Moreover, the present study

reflects in detail the effects of varying non-dimensional parameters such as Knudsen number and normalized wall heat flux on the thermal behavior of flows through micro/nanochannels. Wall boundary effect on the channel mass flux is also reported.

2. Motivation for numerical investigation

The contribution of viscous slip heating on non-equilibrium heat transfer in pressure-driven micro/nanochannels has been evaluated under the constant wall heat flux boundary condition [17]. The reported numerical results showed that the viscous slip heating due to wall shear stress and velocity slip significantly affects the heat transfer process in the rarefied flow. For example, in the case of argon flow in a microchannel with $T_{in} = 400$ K, channel pressure ratio (P_{in}/P_{out}) of 3, $Kn_{in} = 0.05$, $q_w = -25$ W/cm², the DSMC solution predicted a singularity in the Nusselt number (Nu), while the analytical solutions failed to capture this behavior. Based on heat lines shown in Fig. 1, an unusual heat flow pattern is observed in the transverse direction (y); i.e., while cooling boundary condition was applied to the walls, walls heated the flow near the outlet, see Fig. 1. In this occasion, viscous slip heating is of considerable order near the wall, especially as the flow moves towards the channel exit. In this occasion, the net heat flow direction at the centerline was mainly from cold to hot. The Navier-Stokes-Fourier (NSF) equations can not capture this anti-Fourier behavior.

These observations motivated us to investigate the causes influencing the patterns of heat flux lines from the perspective of a particle method. The DSMC method can predict such non-intuitive phenomena over a broad spectrum of Knudsen numbers. However, it cannot provide any further information on the contributing macroscopic terms for this unconventional behavior. Therefore, we employ the constitutive laws of the weakly non-linear form of the Boltzmann equation [3] to find the corresponding macroscopic terms and their contributions to the reported heat flux behavior at low rarefaction conditions.

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