International Journal of Thermal Sciences 98 (2015) 51–59

Contents lists available at ScienceDirect

International Journal of Thermal Sciences

journal homepage: www.elsevier.com/locate/ijts

A new form of the second-order temperature jump boundary condition for the low-speed nanoscale and hypersonic rarefied gas flow simulations

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ARTICLE INFO

Article history:
Received 10 January 2015
Received in revised form
18 June 2015
Accepted 27 June 2015
Available online 26 July 2015

Keywords:
Nanoscale
Hypersonic rarefied gas flow
Second-order jump/slip boundary conditions

ABSTRACT

The accuracy of numerical simulations of rarefied gas flows, in particular the Navier-Stokes-Fourier (N–S–F) equations, depends on the employed surface boundary conditions. In the literature, the combination of the second-order slip/jump conditions has primarily been used for either the Burnett or the BGK Burnett equations for hypersonic gas flows. In this work, we suggest the second-order temperature jump condition in a new form. The second-order slip/jump conditions are implemented in the framework of OpenFOAM to employ with the N–S–F equations for low-speed nanoscale and hypersonic rarefied gas flows. We investigate both the first and second-order slip/jump boundary conditions for low speed rarefied gas flow in the pressure-driven backward facing step nanochannel as well as hypersonic gas flows over the flat plate and past a circular cylinder in cross-flow. Simulation results show that the combination of the second-order slip/jump (in new form) conditions predicts better surface properties than those of the first-order slip/jump conditions for all cases studied by comparing the Burnett and DSMC data. Especially, the N–S–F simulation results of the second-order slip/jump (in new form) conditions of the cylinder case can capture the Burnett data at Kn = 0.1, while those of the first-order conditions do not.

1. Introduction

Translational nonequilibrium of a rarefied gas flow in micro/nano-devices or hypersonic vehicles can be characterized by the Knudsen number, *Kn*, that is the ratio of the molecular mean free path, λ, to the characteristic length of their geometry, *l*. If the gas density is relatively high and *Kn* is small, gas flows may be simulated by solving the Euler ($Kn \leq 0.001$) or the Navier–Stokes–Fourier (N–S–F) equations with no-slip boundary conditions ($0.001 \leq Kn \leq 0.01$). The lack of collisions means the N–S–F equations become inappropriate in rarefied regimes indicated by a large Knudsen number. An approach for improving the N–S–F equations in the range of $0.01 \leq Kn \leq 0.1$, i.e. slip regime, is to use velocity slip and temperature jump boundary conditions. However, when *Kn* rises in the range $0.1 \leq Kn \leq 10$, this is called the transition regime: the N–S–F equations become inappropriate because the near-equilibrium fluid assumption for flows has broken down. For $Kn \geq 10$ this regime is called as the free molecular regime. Nonequilibrium gaseous flows of engineering interest such as the hypersonic rarefied regime and the nanoscale low-speed (creeping) regime in nanodevices are considered in the present work. The high Mach, *Ma*, and Knudsen numbers are the sources of thermal nonequilibrium in both cases. In hypersonic gas flows, the main causes of significant nonequilibrium may be high velocities, high temperatures and the low gas density. A velocity gradient in a viscous fluid will cause a transfer of momentum and a temperature gradient will transport heat energy. The transfers of momentum and energy are due to translational nonequilibrium and appear like the effect of viscosity and thermal conductivity. In Nano Electronic Mechanical Systems(NEMS), fluid mechanics and heat transfer of the gas nano-flows due to nonequilibrium effects such as small characteristic length scale, rarefaction and gas–surface interactions play important roles.

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http://dx.doi.org/10.1016/j.ijthermalsci.2015.06.017
1290-0729/

Many studies of the rarefied gas flow in nano/microscale devices and hypersonic aerodynamics with Direct Simulation Monte Carlo (DSMC) and Computational Fluid Dynamics (CFD) were presented in Refs. [1–12]. A typical CFD method, which solves the N–S–F equations with appropriate surface boundary conditions, may simulate successfully rarefied gas flows in the slip regime, up to a *Kn* of 0.1. This paper will focus on the surface nonequilibrium boundary conditions for the CFD method using the N–S–F equations, and low enthalpy flows where chemical nonequilibrium is not important. The accuracy of the N–S–F simulations depends on that of the surface boundary conditions. Some research reported in Refs. [2,12–29] concerning slip velocity, and temperature jump boundary conditions were reviewed and their advantages and disadvantages were briefly discussed. The first-order conventional slip and jump conditions were developed by Maxwell and Smoluchowski for a flat plate, presented in Refs. [13] and [17], respectively. The Maxwell slip and Smoluchowski jump conditions are pure forms and are expressed by the normal gradients of velocity and temperature at the surface. Another first-order slip condition described by Shen et al. [14] depends not only on the velocity gradient in the surface normal direction, but also on the pressure gradient in the flow direction. Moreover, general slip and jump conditions for a solid surface in rarefied multi-component gas flows, reported by Qazi-Zadeh et al. [15], were developed using the kinetic theory of gasses. Alternative slip and jump conditions developed by Gökçen et al. [16] aim to reduce to the classical Maxwell slip and Smoluchowski jump conditions, and also to yield the correct shear stress and heat transfer of the free molecular flows in the limiting case of very large Knudsen numbers.

Second-order slip boundary conditions for simulating rarefied gas flows were developed for a planar surface in Refs. [2,12,18–26]. They include an additional second-order term of the normal gradient of velocity. The free coefficients of the first-order and second-order terms are still the subject of much discussion. Second-order slip conditions were usually tested for microscale gas flows and good results were obtained. Second-order temperature jump condition was developed from the first-order Smoluchowski jump condition by using a Taylor series expansion of the second-order in Kn [12,25]. Moreover, the second-order jump condition in a simple form was also proposed in Refs. [28,29]. The combination of the second-order jump/slip conditions, which were developed by using a Taylor series expansion, was implemented to work with either the Burnett or the BGK Burnett equations in Ref. [25] for hypersonic gas flows.

The main novelty of this study is to present the derivation for a new form of the second-order temperature jump boundary condition. Although its new form was employed in our recent work [30,31] to simulate some rarefied gas flows, however, there was no derivation in details for its new form in Refs. [30,31]. Here, the coefficients in the second-order jump/slip boundary conditions are numerically investigated to match the DSMC and Burnett data for three different cases: the pressure-driven backward facing step nanochannel [5], hypersonic gas flows past a circular cylinder in cross-flow [25] and over a flat plate [32]. In the present study, we report the extended investigations for the backward facing step nanochannel and flat plate cases which were briefly treated in our conference paper [30].

2. Nonequilibrium boundary conditions

The open source CFD software, OpenFOAM [33], is used in the present work. It uses the finite volume, numeric to solve systems of partial differential equations ascribed on any three-dimensional unstructured mesh of polygonal cells. We use solver *rhoCentralFoam* in OpenFOAM to perform all CFD simulations. In this solver, the N–S–F equations are numerically solved with the high-resolution central scheme described in Ref. [34]. Various slip and jump boundary conditions were implemented into this solver to simulate the rarefied gas flows. Most nonequilibrium slip/jump boundary conditions can be expressed in the form [35,37]:

$$\phi + a(\mathbf{S}\cdot\nabla_n\phi) = \Phi, \tag{1}$$

where $\nabla_n \equiv \mathbf{n}\cdot\nabla$ is the component of the gradient normal to boundary surface; a is the specific coefficient of boundary condition; Φ is the limiting value in the case of no-slip/jump, e.g., the wall velocity or temperature; and φ is variable of interest. Tensor $\mathbf{S} = \mathbf{I}-\mathbf{nn}$, where $\mathbf{n}$ is the unit normal vector defined as positive in the direction pointing out of the flow domain and $\mathbf{I}$ is identity tensor, removes normal components of any non-scalar field, e. g., velocity, so that slip only occurs in the direction tangential to the surface. For temperature, T, the transformation by tensor $\mathbf{S}$ is omitted in equation (1) since T is a scalar that is unaffected by the transformation [37]. The normal gradient can be expressed numerically as:

$$\nabla_n\phi = C_\Delta(\phi - \phi_i), \tag{2}$$

where the subscript "i" denotes a value in the numerical cell adjacent to the boundary face of the solid surface; and $C_\Delta = 1/|\mathbf{d}|$, , with $\mathbf{d}$ the distance from the numerical cell center to the boundary face center of the solid surface.

2.1. Slip and temperature jump boundary conditions in CFD and DSMC

The first-order Maxwell slip boundary condition in Ref. [13], including the effect of thermal creep, can be expressed in vector form as [13,18]:

$$\mathbf{u} = -\left(\frac{2-\sigma_u}{\sigma_u}\right)\frac{\lambda}{\mu}\boldsymbol{\tau} - \frac{3}{4}\frac{\Pr(\gamma-1)}{\gamma p}\mathbf{q} + \mathbf{u}_w, \tag{3}$$

where $\mathbf{u}$ is the velocity; the tangential shear stress is $\boldsymbol{\tau} = \mathbf{S}\cdot(\mathbf{n}\cdot\boldsymbol{\Pi})$ and the heat flux is $\mathbf{q} = \mathbf{Q}\cdot\mathbf{S}$ at the surface. The $\mathbf{Q}$ is the heat flux vector along the surface; $\boldsymbol{\Pi}$ is the stress tensor at the surface; λ is the mean free path; γ is the specific heat ratio; Pr is the Prandtl number; μ is viscosity; p is the pressure and $\mathbf{u}_w$ is the wall velocity. The tangential momentum accommodation coefficient, σ_u, determines the proportion of molecules reflected from the surface specularly (equal to $1 - \sigma_u$) or diffusely (equal to σ_u), and $0 \le \sigma_u \le 1$. Substituting $\boldsymbol{\tau} = \mathbf{S}\cdot(\mathbf{n}\cdot\boldsymbol{\Pi})$ and $\boldsymbol{\Pi} = \mu\nabla\mathbf{u} + \boldsymbol{\Pi}_{mc}$ with $\boldsymbol{\Pi}_{mc} = \mu\left((\nabla\mathbf{u})^T - \left(\frac{2}{3}\right)\mathbf{I}\mathrm{tr}(\nabla\mathbf{u})\right)$ into equation (3), where the superscript T denotes the transpose and tr indicates the trace. Equation (3) becomes [8].

$$\mathbf{u} + \left(\frac{2-\sigma_u}{\sigma_u}\right)\lambda(\mathbf{S}\cdot\nabla_\mathbf{n}\mathbf{u}) = \mathbf{u}_w - \left(\frac{2-\sigma_u}{\sigma_u}\right)\frac{\lambda}{\mu}\mathbf{S}\cdot(\mathbf{n}\cdot\boldsymbol{\Pi}_{mc}) - \frac{3}{4}\frac{\mu}{\rho}\frac{\mathbf{S}\cdot\nabla T}{T}, \tag{4}$$

where ρ is density and T is temperature. The right-hand side of the equation (4) contains three terms that are associated with (in order): the surface velocity, the so-called curvature effect, and thermal creep. The Maxwellian mean free path, λ, is defined as follows [4]:

$$\lambda = \frac{\mu}{\rho}\sqrt{\frac{\pi}{2RT}}, \tag{5}$$