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Numerical Validation of Brenner's Hydrodynamic Model by Force Driven Poiseuille Flow

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Abstract. Recently Brenner [Physica A **349**, 60 (2005)] proposed a modified Navier-Stokes set of equations. Based on some theoretical arguments and some limited experiments, the model is expected to be able to describe flows with a finite Knudsen number. In this work, we apply this model to the plane Poiseuille flow driven by a force, and compare the results with the Direct Simulation Monte Carlo (DSMC) measurements. It is found that Brenner's model is inadequate for flows with a finite Knudsen number.

AMS subject classifications: 76A02, 76P05, 82C21
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1 Introduction

The Navier-Stokes (NS) set of equations is a sound and robust theoretical model for continuum fluid dynamics where the local thermodynamic equilibrium assumption holds. Although the NS model has gained much successes in many applications, it encounters some challenging difficulties for non-continuum flows which exhibit a finite Knudsen number Kn defined as Kn$=\lambda/H$, where λ is the mean-free-path of the gas and H is a characteristic length of the flow. Non-continuum flows have been widely studied in the rarefied gas community, where the gas density is usually very low so that the mean-free-path of the gas is relatively large. In recent years, non-continuum flows with a normal gas density but with a small characteristic length have also attracted much attention with the rapid development in microelectromechanical systems. Due to the finite Knudsen number effect, the continuum-equilibrium assumption may break down and the NS model will fail to work for these flows [1, 2].

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Some hydrodynamic models beyond the NS equations, such as the Burnett equations, super-Burnett equations, and 13-moments equations, have been proposed from different viewpoints [3–10].

These extended hydrodynamic models are usually derived from gas kinetic theory (the Boltzmann equation) [11]. Unfortunately, these extended continuum models are exposed to some criticisms [12], such as the validity of the Chapman-Enskog expansion for large Kn, the difficulties in ascertaining the boundary conditions, and the inherent instabilities. What is more disappointing is that most of these higher-order models cannot even describe the simple Kramer's problem correctly [13].

Owing to the difficulties arising in the non-Navier-Stokes hydrodynamic models, there are increasing interests to rescue the NS model for non-continuum flows in recent years [14–20]. These models are still in the NS framework, and share most of the advantages of the NS model such as the simple structure and the easy implementation. Recently, Brenner proposed one such model based on a new picture of the fluid velocity [21–23], which we will term as "Brenner-Navier-Stokes" (BNS) model in this work. Compared with other extended hydrodynamics models derived from the Boltzmann equation, the BNS is much simpler because only one single additional term is introduced into each of the momentum and energy equations. Furthermore, although the BNS model was derived phenomenologically, there are some independent experimental and theoretical evidences that it has the potential to model non-continuum flows [21,22,24–26].

However, as a new hydrodynamic model the BNS equations should be tested by some well-accepted benchmark problems before acceptance. In this work, we will investigate the applicability of the BNS model for rarefied gas flows with a small but finite Knudsen number (Kn$\leq$0.1). The test problem employed here is a force driven Poiseuille flow between two parallel plates. Both Direct Simulation Monte Carlo (DSMC) and kinetic theory have shown that even with a small Kn, the pressure and temperature profiles in this flow exhibit qualitatively different behaviors from those predicted by the NS equations [27–31]. Therefore, this flow can serve as a good test problem for any extended hydrodynamic models intended for non-continuum flows.

2 The Brenner-Navier-Stokes equations

Generally, the hydrodynamic equations that govern the fluid motion can be expressed as

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}_m) = 0, \tag{2.1}$$

$$\frac{\partial (\rho \boldsymbol{u}_m)}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}_m \boldsymbol{u}_m) - \boldsymbol{\nabla} \cdot \boldsymbol{P} = \rho \boldsymbol{a}, \tag{2.2}$$

$$\frac{\partial (\rho e)}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u}_m e) + \boldsymbol{\nabla} \cdot \boldsymbol{j}_e - \boldsymbol{\nabla} \cdot (\boldsymbol{P} \cdot \boldsymbol{u}_m) = \rho \boldsymbol{a} \cdot \boldsymbol{u}_m, \tag{2.3}$$

where ρ is the mass density, $\boldsymbol{u}_m$ the mass velocity, $e=\epsilon+\boldsymbol{u}_m^2/2$ the specific total energy with ϵ the internal energy, $\boldsymbol{j}_e$ the flux for the internal energy, $\boldsymbol{a}$ the acceleration, and $\boldsymbol{P}=-p\boldsymbol{I}+\boldsymbol{\tau}$ the pressure tensor, where $\boldsymbol{\tau}$ is the viscous stress tensor given by

$$\boldsymbol{\tau}=2\mu\overset{\circ}{\boldsymbol{D}}+\kappa(\nabla\cdot\boldsymbol{u})\boldsymbol{I}, \tag{2.4}$$

where $\overset{\circ}{\boldsymbol{D}}=\boldsymbol{D}-\frac{1}{3}\mathrm{tr}(\boldsymbol{D})\boldsymbol{I}$ with $\boldsymbol{D}=\frac{1}{2}[\nabla\boldsymbol{u}+(\nabla\boldsymbol{u})^{\mathsf{T}}]$, and μ and κ are the shear and bulk viscosities, respectively. The internal energy flux $\boldsymbol{j}_e$ in the energy equation is specified according to the Fourier law, i.e.,

$$\boldsymbol{j}_e=-k\nabla T, \tag{2.5}$$

where k is the thermal conductivity and T is the temperature.

In the classical NS model, the velocity $\boldsymbol{u}$ in the constitutive equation (2.4) is taken to be the mass velocity $\boldsymbol{u}_m$. Recently, Brenner argued that this well-accepted choice may be invalid. He recognized that a deformable fluid element consisting of a large set of molecules may behave differently from a rigid body, and macroscopic fluid movement can occur purely diffusively by the movement of volume without a convective movement of mass. Consequently, the fluid's Lagrangian velocity may differ from its Eulerian or mass velocity. Based on this realization, Brenner argued that it was necessary to include the volume diffusive effect in the momentum equation.

The key point of Brenner's modification to the NS equations is to use the volume velocity $\boldsymbol{u}_v$ instead of the mass velocity $\boldsymbol{u}_m$ in the Newton's viscosity law, which relates to the flux of volume rather than mass [21–23]. These two velocities are not independent, but are related as

$$\boldsymbol{u}_v=\boldsymbol{u}_m+\boldsymbol{j}_v, \tag{2.6}$$

where $\boldsymbol{j}_v$ is the diffusive volume flux. In the case of single-component fluids undergoing heat transfer, Brenner proposed a constitutive equation for $\boldsymbol{j}_v$ [21,22]:

$$\boldsymbol{j}_v=\alpha_v\nabla\ln\rho, \tag{2.7}$$

where α_v is the volume diffusivity. How α_v should be quantified for a given fluid state is an open question. In the original work of Brenner [21,22], α_v is directly identified to be the thermal diffusivity $\alpha=k/\rho c_p$, where c_p the isobaric specific heat. However, recently Greenshields and Reese found that this choice of α_v would produce some unphysical results in their study of shock structure [26]. Instead, they argued that α_v should take the value of the kinematic viscosity $\nu=\mu/\rho$.

Some other formulations for $\boldsymbol{j}_v$ were also proposed in the literature. For instances, Öttinger proposed a more general formulation [32,33]:

$$\boldsymbol{j}_v=\frac{D}{\rho}\left[\nabla\left(\frac{\mu_c}{T}\right)-\alpha'\nabla\left(\frac{1}{T}\right)\right]=\frac{D}{\rho^2}\left[\nabla\left(\frac{p}{T}\right)+\rho(\epsilon-\alpha')\nabla\left(\frac{1}{T}\right)\right], \tag{2.8}$$

where $D=\rho\alpha_v/R$ is the diffusion coefficient with R the gas constant, μ_c is the chemical potential, and α' is a coupling coefficient between mass and heat fluxes. As $\alpha'=\epsilon$, the

mass diffusion is driven by the density, and Eq. (2.8) reduces to Eq. (2.7) for an ideal gas; as $\alpha'=\epsilon+RT$, the driven force for the mass diffusion is the pressure gradient, and $j_v=\alpha_v\nabla\ln p$.

The internal energy flux $\boldsymbol{j}_e$ in the BNS model is also modified to include the contribution of the volume flux:

$$\boldsymbol{j}_e=-k\nabla T-p\boldsymbol{j}_v. \tag{2.9}$$

With Eq. (2.4) together with Eqs. (2.8) and (2.9), the Brenner-Navier-Stokes equations are closed. But it should be pointed that the BNS equations can also be expressed in terms of the velocity $\boldsymbol{u}_v$, which have been used in [21,22,25,32,33].

3 Description of the force-driven Poiseuille flow

We consider the force-driven Poiseuille flow between two parallel plates located at $y=\pm H/2$. The flow is assumed to be unidirectional, i.e., $\partial_x\phi=0$ for any variable ϕ, and the velocity has only an x-component in the laminar and stationary case, i.e., $\boldsymbol{u}_m=(u,0,0)$. Under such conditions, the BNS equations become

$$\frac{d}{dy}\left(\mu\frac{du}{dy}\right)+\rho a=0, \tag{3.1}$$

$$\frac{d}{dy}\Big[-p+\left(\kappa+\frac{4}{3}\mu\right)\frac{dj_y}{dy}\Big]=0, \tag{3.2}$$

$$\frac{d}{dy}\left(k\frac{dT}{dy}+pj_y\right)+\mu\left(\frac{du}{dy}\right)^2=0, \tag{3.3}$$

where j_y is the y-component of $\boldsymbol{j}_v$ given by Eq. (2.8). In the case of classical NS model, $j_y=0$ and Eq. (3.2) always gives a constant pressure. For the BNS model, however, j_y is nonzero in general, and thus a non-constant pressure can be expected.

By introducing the following variables: $Y_1=\rho$, $Y_2=u$, $Y_3=T$, $Y_4=j_y$, $Y_5=\mu du/dy$, and $Y_6=kdT/dy+pj_y$, the system (3.1)-(3.3) can be rewritten as a system of six coupled first-order differential equations,

$$\frac{d\boldsymbol{Y}}{dy}=\boldsymbol{F}(\boldsymbol{Y}), \tag{3.4}$$

where

$$\boldsymbol{F}(\boldsymbol{Y})=\begin{bmatrix} Y_1Y_4/\alpha+Y_1Z(c_vY_3-\alpha')/RY_3^2 \\ Y_5/\mu \\ Z \\ (c+RY_1Y_3)/(\kappa+\frac{4}{3}\mu) \\ -Y_1a \\ -Y_5^2/\mu \end{bmatrix}, \tag{3.5}$$

with c being the integral constant of Eq. (3.2), c_v the specific heat at constant volume, and

$$Z=(Y_6-RY_1Y_3Y_4)/k.$$

In the above formulation we have assumed that the fluid is an ideal gas, i.e., $p=\rho RT$.

The above system contains seven unknowns ($Y_1 \sim Y_6$ and c). In order to solve the system, suitable boundary conditions must be supplemented. However, the issue of boundary conditions for the BNS equations is still an unresolved problem. This is actually another challenging task. However, rather than looking at this point in a general setting, it is important to know first if the BNS model can indeed reproduce the basic features of the flow. Therefore, in order to avoid the difficulty of specifying boundary conditions, we make use of the symmetric property of the flow, i.e.,

$$\left.\frac{du}{dy}\right|_{y=0} = \left.\frac{d\rho}{dy}\right|_{y=0} = \left.\frac{dT}{dy}\right|_{y=0} = 0, \tag{3.6}$$

and use the centerline ($y=0$) values measured in the Direct Simulation Monte-Carlo (DSMC) as another three conditions:

$$u(y=0)=u_c, \quad \rho(y=0)=\rho_c, \quad T(y=0)=T_c, \tag{3.7}$$

where u_c, p_c, and T_c are the corresponding DSMC results at the centerline. To close the system (3.4) one more condition is required. To this end, we can set one of the three variables (u, ρ, and T) at $y=-H/2$ to be the corresponding DSMC value. In this way the question of boundary conditions at the solid wall is bypassed, but the calculated velocity profile allows us to compare it with the DSMC results.

4 Results and discussions

In order to make a comparison with the DSMC data reported in [30], here we use the same set-up as that used in the DSMC: the fluid is an ideal gas consisting of hard-sphere molecules with unit mass ($m=1$) and unit diameter ($d=1$); At a reference density $\rho_0=1.21\times10^{-3}$, the mean-free-path of the gas is $\lambda=186$; The distance between the two plates is $H=10\lambda$, and the temperatures of the two walls are kept at $T_0=1$; The reference fluid speed is $u_0=\sqrt{2RT_0}=1$, so the gas constant is taken as $R=1/2$; The reference sound speed is $c_s=\sqrt{\gamma RT_0}=0.91$ since the specific heat ratio $\gamma=5/3$ for a monatomic gas; The driven force is set to be $\rho_0 a=8.31\times10^{-8}$.

The Knudsen number of the system considered is 0.1. With so small Kn, it is generally thought that the NS equations with a slip boundary condition can be used to describe the flow and heat transfer behaviors. However, some previous studies [27–31] have revealed that even for this simple case with the relative small Knudsen number, the NS equations still failed to predict a qualitative correct solution. Specifically, the NS equations cannot capture the central minimum in the temperature profile and a non-constant pressure profiles in the cross-section, which are both predicted by the kinetic theory and observed in the DSMC simulations. Unlike the slip phenomena, the discrepancy is not just near a boundary, but throughout the system. Furthermore, as pointed out by Xu and Li [31] that it is impossible to correct this failure by modifying the equation of state, transport coefficients or boundary conditions within the NS framework.

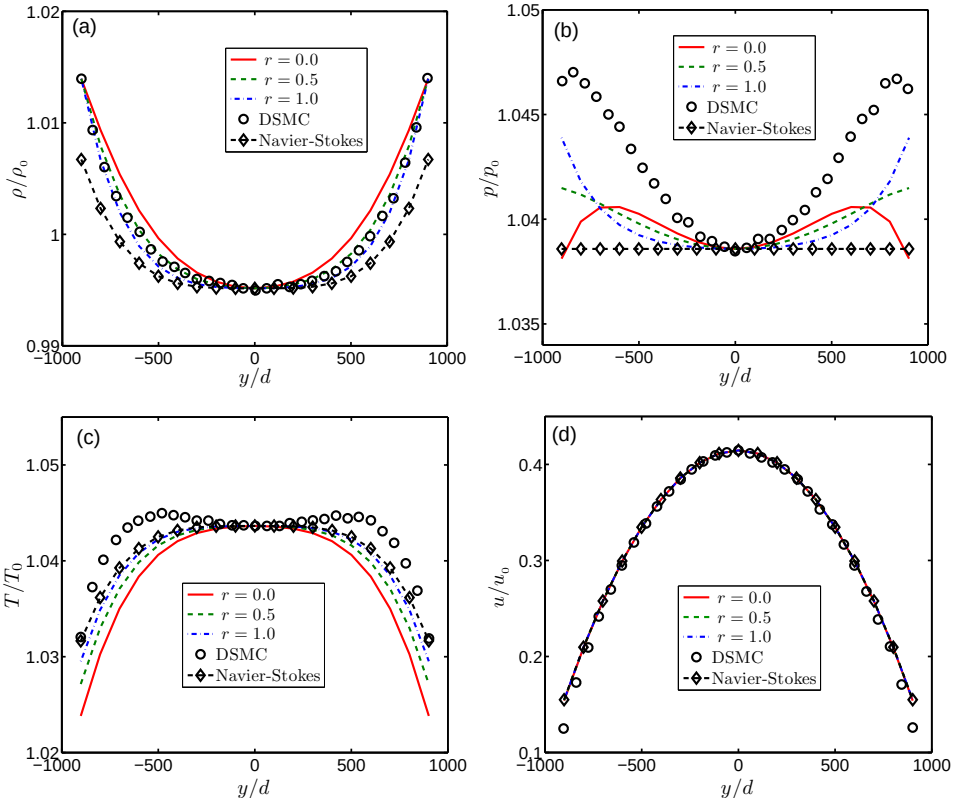

Figure 1: (Color online) The density (a), pressure (b), temperature (c), and velocity (d) profiles of the force-driven Poiseuille flow with different coupling parameter $\alpha'=\epsilon+rRT$ ($\alpha_v=\alpha$).

Now we see whether the Brenner-Navier-Stokes equations can yield improved results for this problem. The system of the six first-order differential equations (3.4) is solved under the conditions (3.6) and (3.7) together with a supplemental condition $\rho(-H/2)=\rho_b$, where ρ_b is the value of the density at the bottom plate measured from the DSMC data. The numerical method employed here is the ODE (Ordinary-Differential-Equation) solver in the Matlab software. The solver uses an adaptive mesh and thus can give a very accurate solution.

First, we test the BNS equations with $\alpha_v=\alpha$ in $\boldsymbol{j}_v$ as suggested by Brenner [21,22]. The coupling parameter α' in Eq. (2.8) is adjusted according to $\alpha'=\epsilon+rRT$ by changing r from 0 to 1.0. The results are shown and compared with the DSMC data [30] and the solutions of the classical NS equations in Fig. 1. It can be seen that the density and velocity profiles (Figs. 1(a) and 1(d)) are comparable to the DSMC and NS results in all cases; Particularly, the velocity profiles at different r are actually indistinguishable from the NS solution. Actually, the differences among the velocities are within the machine accuracy. The pressure and temperature profiles of the BNS model, however, demonstrate some clear parameter-dependent deviations from the DSMC results (Figs. 1(b) and 1(c)). Specifically, the NS model gives a constant pressure, while the pressure profiles of the BNS model are non-constant in all cases, which are in qualita-

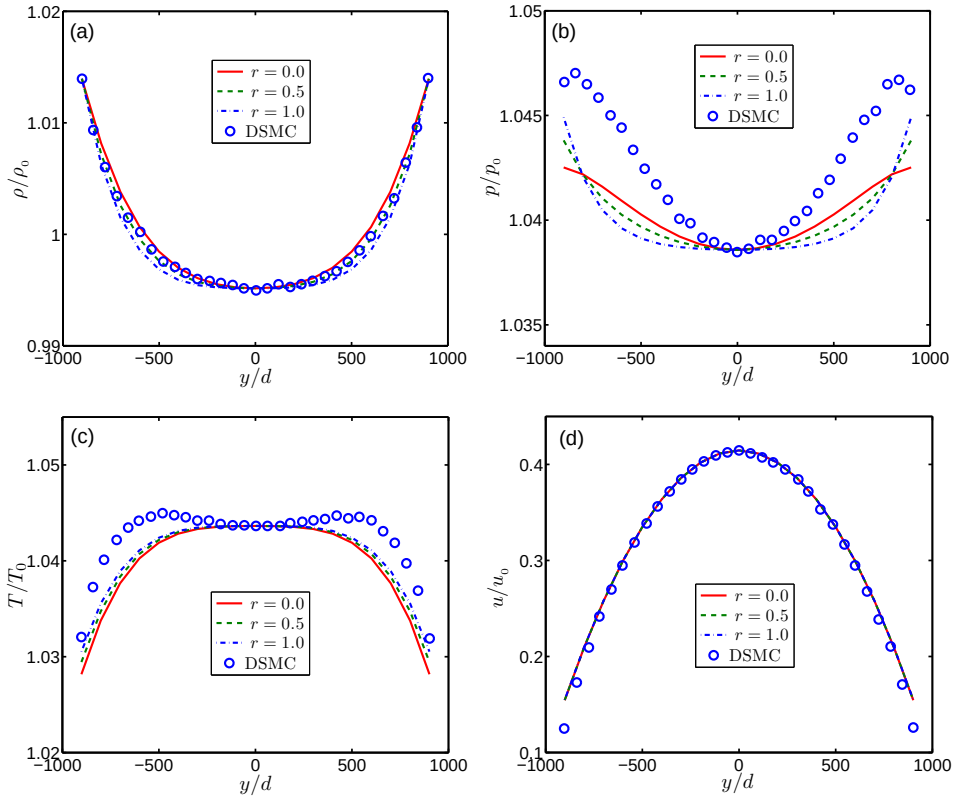

Figure 2: (Color online) The density (a), pressure (b), temperature (c), and velocity (d) profiles of the force-driven Poiseuille flow with different coupling parameter $\alpha'=\epsilon+rRT$ ($\alpha_v=\nu$).

tive agreement with the DSMC results. The local minimum in pressure in the channel center is also captured successfully in each case. Particularly, as r=0, i.e., the mass diffusion is driven by the density gradient $\nabla\rho$, the two local maxima near the walls are also obtained. However, in contrast to the DSMC results, it is found that the pressure value at the wall is lower than the central minimum. With the increase in r, the pressure gradient becomes more dominating in the mass diffusion, and the pressure at the wall becomes more close to the DSMC data, but the near-wall local maxima disappear. Regarding the temperature field, it is seen from Fig. 1(c) that none of profiles exhibits the bimodal structure of the DSMC result. This qualitative discrepancy indicates that the BNS equations are still not adequate for the present flow, although it can give an improved pressure prediction.

We also tested the BNS model with α_v=ν, which was suggested by Greenshields and Reese [26]. The numerical results are shown in Fig. 2. Generally, the results are very similarly to those shown in Fig. 1 for α_v=α. But some small differences are observed in the pressure and temperature profiles (Figs. 2(b) and (c)): In this case, both the pressure and temperature at the walls become larger than the corresponding values in the case of α_v=α. Particularly, the pressure distribution as r=0 is more close to the DSMC data now. These results confirm the claim made by Greenshields and

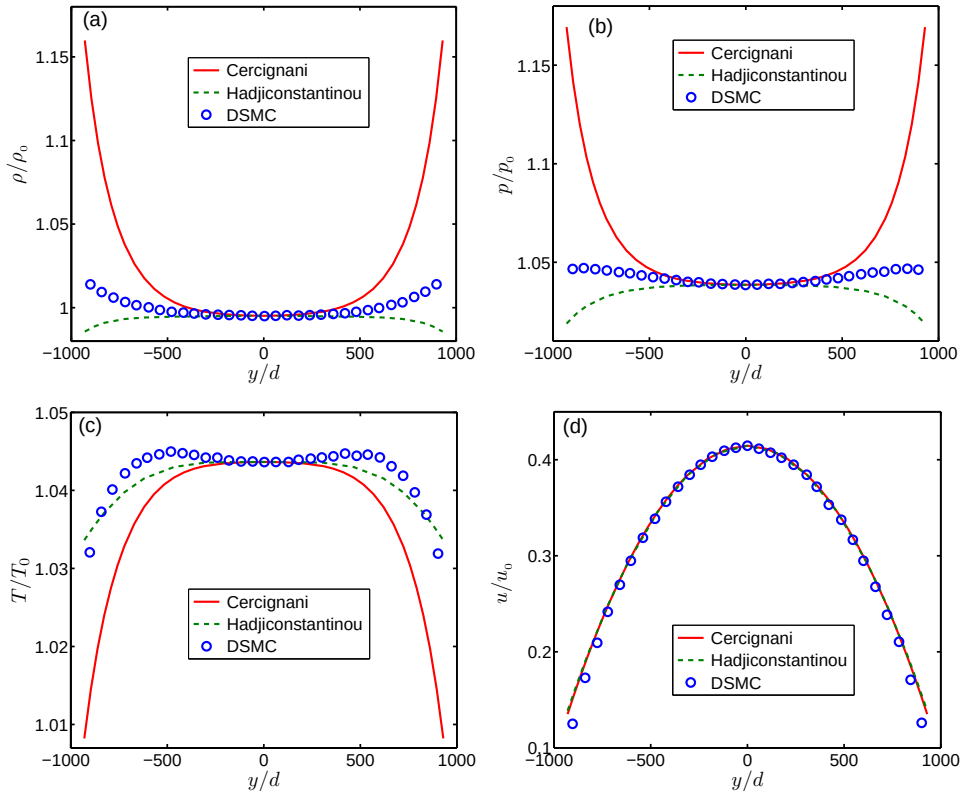

Figure 3: (Color online) The density (a), pressure (b), temperature (c), and velocity (d) profiles of the force-driven Poiseuille flow with the slip boundary condition 4.1 ($\alpha'=\epsilon+RT$ and $\alpha_v=\nu$).

Reese [26] in the study of shock structure that it may be more appropriate to take $\alpha_v=\nu$ than to take $\alpha_v=\alpha$. We also tested the model with other values of α_v and α', and similar results are obtained. These facts show that the change of the model parameters cannot alter the fundamental properties of the BNS equations.

We also tested the structure of the Poiseuille flow with other boundary conditions. For instance, a slip velocity boundary,

$$u_s \equiv u(b) - u_w = A_1\lambda\frac{du}{dy}\bigg|_w - A_2\lambda^2\frac{du^2}{dy^2}\bigg|_w, \tag{4.1}$$

is employed as a supplemental condition in addition to (3.6) and (3.7). Here $u(b)$ is the gas velocity at the wall, u_w is the wall velocity, A_1 and A_2 are two slip coefficients characterizing the gas-wall interaction. For a fully diffusive wall, Cercignani [11] obtained from the solution of the Boltzmann BGK equation that $A_1\approx1.146$ and $A_2\approx0.979$, while later Hadjiconstantinou [34] proposed an improved version, $A_1\approx1.11$ and $A_2\approx0.61$. In Fig. 3, the profiles of the density, pressure, temperature, and velocity are shown for the two sets of parameters. Here we take $\alpha=\nu$ and $\alpha'=\epsilon+RT$. As shown, in both cases the velocity profiles are still similar to those in Figs. 1 and 2, which indicates that the velocity is insensitive to boundary conditions. On the other hand, the density,

pressure, and temperature are closely dependent on the slip coefficients. Specifically, the tendencies of density and pressure of Cercignani's slip boundary condition are qualitatively in agreement with the DSMC data, while those of Hadjiconstantinou's boundary condition are incorrect qualitatively. But the temperature profiles in both cases are similar to those shown in Figs. 1 and 2: the bimodal structure is not capture. These results confirm again that the BNS model is not adequate for capturing the basic structure of the Poiseuille flow with a finite Knudsen number regardless of boundary conditions.

5 Summary

We have applied the BNS equations to the planar force-driven Poiseuille flow with different parameters, and compared the results with the DSMC data and the NS solutions. It is found that the BNS model can yield some improved predictions in comparison with the classical NS model, especially in the pressure field. However, the BNS model cannot give a qualitatively correct temperature profile. This fact shows that the Brenner's hydrodynamic model is still not adequate for describing gaseous micro flows. This failure is expectable: As pointed out by Brenner [21, 22], the additional term appearing in the Newton's law can be viewed as a term in the Burnett stress resulting from the Boltzmann equation in the Chapman-Enskog analysis. However, as shown in some previous studies [31, 35, 36], the Burnett equations are not able to capture the bimodal temperature profile of the force-driven Poiseuille flow, which can only be reproduced at the super-Burnett order [36]. The linkage to the Burnett equations also implies that specifying suitable boundary conditions for the BNS equations is another challenging problem for further applications, which has been bypassed in this work. Actually, this fact has been pointed out theoretically in [29], where the problem of the boundary condition was solved by the asymptotic expansion. In [29], it was also shown that the discrepancy from the Navier-Stokes equation manifests itself at the second order in the Knudsen number, which can also be observed in Figs. 1 and 2, where the differences between the DSMC and Navier-Stokes results are of the order of Kn^2=0.01.

It is noted that more sophisticated versions of the BNS model have been suggested recently [32, 33, 37]. We would like to emphasize here that the formulation (2.8) used in the present study is taken from [32, 33], which is already a generalized version of Brenner's model, and the present study provide a benchmark for this new type of hydrodynamic model for non-equilibrium flows.

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