

## Super-Burnett solutions for Poiseuille flow

Kun Xu<sup>a)</sup>

Mathematics Department, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong

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In the slip flow regime with  $\text{Kn}=0.1$  for the force and pressure driven Poiseuille flow, Zheng *et al.* [*Rarefied Gas Dynamics*, Vol. 23 (Whistler, Canada, 2002)] found out that the Navier–Stokes equations with slip boundary condition could give qualitative different results in the cross-stream direction from the reliable direct simulation Monte Carlo (DSMC) solution. In this Brief Communication, we are going to show that the discrepancy between the Navier–Stokes and the DSMC results can be resolved based on the simulation results of higher-order equations, such as Burnett and super-Burnett ones. © 2003 American Institute of Physics. [DOI: 10.1063/1.1577564]

It is generally recognized that in the slip flow regime with Knudsen number  $\text{Kn}\leq 0.1$ , the Navier–Stokes equations with the slip boundary condition is capable to accurately simulate the microchannel flow. However, for the simple force and pressure driven Poiseuille flow in the slip flow regime with relative small gradient and Knudsen number, the Navier–Stokes equations give qualitatively incorrect predictions.<sup>1,2</sup> For example, they fail to reproduce the central minimum in the temperature profile and nonconstant pressure profile, which are both predicted by the kinetic theory and observed in the direct simulation Monte Carlo (DSMC) simulations.<sup>3–7</sup> For the pressure driven case, in the cross-stream direction, Zheng *et al.* even found that the curves in the pressure distribution of the Navier–Stokes solutions are opposite in comparison with the DSMC result.<sup>1</sup> In order to understand these phenomena, many analyses have been done. For example, in the force driven case the nonconstant pressure is well explained based on the Burnett equations,<sup>5</sup> but the temperature minimum at the center is explained only through the kinetic theory.<sup>3,4,7</sup> For the pressure driven case, basically no analysis has been done yet.

In order to further understand these phenomena, in this Brief Communication the BGK-Burnett and BGK-super-Burnett schemes will be used to study the Poiseuille flow, and to explain the source for the abnormal behavior in the temperature and pressure distributions. It will be shown that the temperature minimum in the force driven case is generated by the super Burnett order and the opposite curves between the Navier–Stokes and DSMC solutions in the pressure driven case can be resolved on the Burnett order. In the following, we are going to present the numerical schemes and the simulation results.

The BGK-Burnett and super Burnett schemes are the extension of the finite volume gas-kinetic BGK method.<sup>8</sup> For the 2D Poiseuille flow, a directional splitting gas-kinetic scheme will be used to solve the BGK model<sup>9</sup> in each direction separately. For example, in the  $x$  direction, the BGK model is

$$f_t + uf_x = \frac{g-f}{\tau}, \quad (1)$$

where  $f$  is the gas distribution function and  $g$  is the equilibrium state approached by  $f$ . Both  $f$  and  $g$  are functions of space  $x$ , time  $t$ , particle velocities  $(u, v)$ , and internal variable  $\xi$ . The particle collision time  $\tau$  is related to the viscosity and heat conduction coefficients. The equilibrium state is a Maxwellian distribution

$$g = \rho \left( \frac{\lambda}{\pi} \right)^{(K+2)/2} e^{-\lambda((u-U)^2 + (v-V)^2 + \xi^2)}$$

where  $\rho$  is the density,  $U$  and  $V$  are the macroscopic velocities in the  $x$  and  $y$  directions, and  $\lambda = m/2kT$ , where  $m$  is the molecular mass,  $k$  is the Boltzmann constant, and  $T$  is the temperature. In the equilibrium state,  $K$  is the internal degree of freedom. For example, for a monatomic gas in the 2D Poiseuille flow,  $K$  is equal to 1 to account for the particle motion in the  $z$  direction.

The relation between mass  $\rho$ , momentum  $(\rho U, \rho V)$ , and energy  $\rho E$  densities with the distribution function  $f$  is

$$(\rho, \rho U, \rho V, \rho E)^T = \int \psi_\alpha f d\Xi, \quad \alpha = 1, 2, 3, 4, \quad (2)$$

where  $\psi_\alpha$  is the component of the vector of moments

$$(\psi_1, \psi_2, \psi_3, \psi_4)^T = (1, u, v, \frac{1}{2}(u^2 + v^2 + \xi^2))^T,$$

and  $d\Xi = dudvd\xi$  is the volume element in the phase space with  $d\xi = d\xi_1 d\xi_2 \dots d\xi_K$ . Since mass, momentum and energy are conserved during particle collisions,  $f$  and  $g$  satisfy the conservation constraint

$$\int (g-f)\psi_\alpha d\Xi = 0, \quad \alpha = 1, 2, 3, 4. \quad (3)$$

The general solution  $f$  of the BGK model (1) at a cell interface  $x_{j+1/2}$  and time  $t$  is

$$f(x_{j+1/2}, t, u, v, \xi) = \frac{1}{\tau} \int_0^t g(x', t', u, v, \xi) e^{-(t-t')/\tau} dt' + e^{-t/\tau} f_0(x_{j+1/2} - ut), \quad (4)$$

<sup>a)</sup>Fax: (852)2358-1643. Electronic mail: makxu@uxmail.ust.hk

where  $x' = x_{j+1/2} - u(t - t')$  is the particle trajectory and  $f_0$  is the initial gas distribution function  $f$  at the beginning of each time step ( $t=0$ ). In order to simplify the notation,  $x_{j+1/2}=0$  will be used in the following text.

The BGK-super Burnett scheme is based on the above integral solution with the construction of an initial nonequilibrium states  $f_0$  up to the super Burnett order, i.e.,  $f_0 = g + \epsilon_1 f_1 + \epsilon^2 f_2 + \epsilon^3 f_3$ . With the introduction of the following notations for the derivatives of a Maxwellian distribution function  $g$ , i.e.,  $g_x = ag$ ,  $g_t = Ag$ ,  $g_{xx} = (a^2 + b)g$ ,  $g_{xt} = (aA + C)g$ ,  $g_{tt} = (A^2 + B)g$ ,  $g_{xxx} = (a^3 + 3ab + d)g$ ,  $g_{xxt} = (A(a^2 + b) + 2aC + F)g$ ,  $g_{xtt} = (aA^2 + 2AC + aB + G)g$ ,  $g_{ttt} = (A^3 + 3AB + E)g$ , all parameters  $a, A, b, B, C, d, E, F, G$  have the functional dependences on  $(1, u, v, \frac{1}{2}(u^2 + v^2 + \xi^2))$ , such that  $q = q_1 + q_2 u + q_3 v + q_4(u^2 + v^2 + \xi^2)$ . From the initially interpolated macroscopic flow variables  $w$  around a cell interface, we can determine  $f_0$  through the relation

$$w_0 + w_1 x + \frac{1}{2} w_2 x^2 + \frac{1}{6} w_3 x^3 = \int f_0 \psi_\alpha d\Xi, \quad \alpha = 1, 2, 3, 4,$$

where  $w_0, w_1, w_2$ , and  $w_3$  are all vectors with four components to account for the mass,  $x$ -momentum,  $y$ -momentum, and energy densities at the location of cell interface, and their first, second, and third order spatial derivatives. In order to further simplify the notation, let us define  $\langle \dots \rangle$  as the moments of the Maxwellian

$$\langle \dots \rangle = \int (\dots) \psi_\alpha g(0,0) d\Xi, \quad \text{for } \alpha = 1, 2, 3, 4.$$

Then, the equilibrium state  $g(0,0)$  at the cell interface can be determined by

$$w_0 = \int \psi_\alpha g(0,0) d\Xi = \langle 1 \rangle.$$

Consequently, the parameters  $a$ ,  $b$ , and  $d$  can be found from

$$\langle a \rangle = w_1, \quad \langle b + a^2 \rangle = w_2, \quad \langle d + a^3 + 3ab \rangle = w_3.$$

After having  $a$ ,  $b$  and  $d$ , based on the condition on the Chapman-Enskog expansion, such as  $\langle \epsilon f_1 \rangle = 0$ ,  $\langle \epsilon^2 f_2 \rangle = 0$ , and  $\langle \epsilon^3 f_3 \rangle = 0$ , we have

$$\langle A + ua \rangle = 0,$$

$$\langle C + aA + u(a^2 + b) \rangle = 0,$$

$$\langle B + A^2 + 2u(aA + C) + u^2(a^2 + b) \rangle = 0,$$

$$\langle F + A(a^2 + b) + 2aC + u(a^3 + 3ab + d) \rangle = 0,$$

$$\langle G + aA^2 + 2AC + aB + 2u(A(a^2 + b) + 2aC + F) + u^2(a^3 + 3ab + d) \rangle = 0,$$

$$\langle E + A^3 + 3AB + 3u(a(A^2 + B) + 2AC + G) + 3u^2(A(a^2 + b) + 2aC + F) + u^3(a^3 + 3ab + d) \rangle = 0,$$

from which the parameters  $A$ ,  $C$ ,  $B$ ,  $F$ ,  $G$ , and  $E$  are uniquely obtained. Then, the integral solution of the BGK model goes to

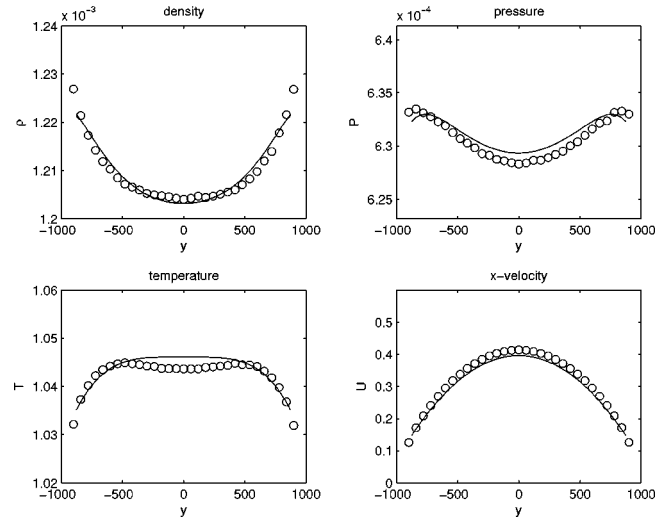


FIG. 1. Flow distribution in the cross-stream direction in the external force driven case. Circles: DSMC results (Ref. 1), solid lines: BGK-Burnett solution.

$$f(0,t) = g(0,0) [1 - \tau au + (-\tau + t)A + (\tau^2 - \tau t + t^2/2) \times (A^2 + B) + (2\tau^2 - \tau t)(aA + C)u + \tau^2(a^2 + b)u^2 + (-\tau^3 + t^3/6 + \tau^2 t - \tau t^2/2)(A^3 + 3AB + E) + (-3\tau^3 + 2\tau^2 t - \tau t^2/2)(aA^2 + 2AC + aB + G)u + (-3\tau^3 + \tau^2 t)(a^2 A + Ab + 2aC + F)u^2 - \tau^3 u^3(a^3 + 3ab + d)]. \quad (5)$$

The particle collision time  $\tau$  is given by  $\tau = \mu/p$ , where  $\mu$  and  $p$  are local dynamical viscosity coefficient and pressure. The above distribution is used for the flux evaluation in the BGK-super Burnett scheme. For the BGK-Burnett scheme, only the terms up to  $\tau^2(a^2 + b)u^2 g$  are used. Due to the Prandtl number fix based on the modification of heat flux,<sup>8</sup> the above scheme solves the Burnett and super Burnett equations with a realistic Prandtl number, such as  $Pr = 2/3$  for a monatomic gas. The diffusion boundary condition is applied based on the incoming mass flux from Eq. (5) and re-emitting them with the wall temperature. All steady state solutions are obtained from the above time-accurate flow solver.

The set up of both external force and pressure driven Poiseuille flow cases is given in Ref. 1. The simulation fluid is a hard-sphere gas with particle mass  $m = 1$  and diameter  $d = 1$ . At the reference density of  $\rho_0 = 1.21 \times 10^{-3}$ , the mean free path is  $l_0 = m(\sqrt{2}\pi\rho_0 d^2)^{-1} = 186$ . The distance between the thermal walls is  $L_y = 10l_0$  and their temperature is  $T_0 = 1.0$ . The reference fluid speed is  $U_0 = \sqrt{2kT_0/m} = 1$  so Boltzmann constant is taken as  $k = 1/2$ . The reference sound speed is  $c_0 = \sqrt{\gamma kT_0/m} = 1$  with  $\gamma = 5/3$  for a monatomic gas. The reference pressure is  $p_0 = \rho_0 kT_0/m = 6.05 \times 10^{-4}$ . The acceleration and pressure gradients are chosen so that the flow will be sub-sonic, laminar and of similar magnitude in the two cases. Specifically,  $\rho_0 f = 8.31 \times 10^{-8}$  for the acceleration-driven case and  $dp/dx = 1.08 \times 10^{-7}$  for the pressure-driven case. In both cases the Knudsen number is

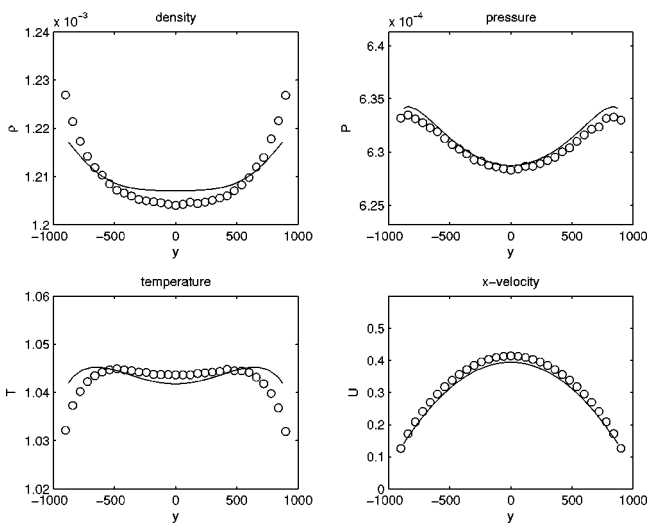


FIG. 2. Flow distribution in the cross-stream direction in the external force driven case. Circles: DSMC results (Ref. 1), solid lines: BGK super-Burnett solution.

$Kn=l_0/L_y=0.1$  and the Reynolds number is of order one. In all calculations, the cell side takes the size of half of the mean free path in the initial data.

For the Navier–Stokes solution, in the force driven case the pressure is a constant in the cross-stream direction.<sup>1</sup> Figure 1 presents the results from the BGK-Burnett solver, the curved pressure distribution is well captured. But, the temperature minimum can be only obtained by the BGK-super-Burnett scheme, which is shown in Fig. 2. This is consistent with the analysis in Ref. 5, where the temperature dip does not appear in the Burnett solution. As the gas rarefaction is increased to  $Kn=0.2$  by reducing the channel height, the temperature dip in the super-Burnett solution is more obvious. See Fig. 3.

For the pressure driven case, the Navier–Stokes and the DSMC results have opposite curves in the pressure distribution in the cross-stream direction,<sup>1</sup> such as that shown in Fig. 4. This phenomena is irrelevant with the slip boundary condition or the constitutive relations. Figure 5 is the result calculated by the BGK-Burnett scheme, where the pressure distribution is basically consistent with DSMC solution. Figure 6 shows the BGK-super-Burnett solution, which matches the DSMC result perfectly.

This Brief Communication shows that in the slip flow regime the abnormal phenomena between the DSMC and the

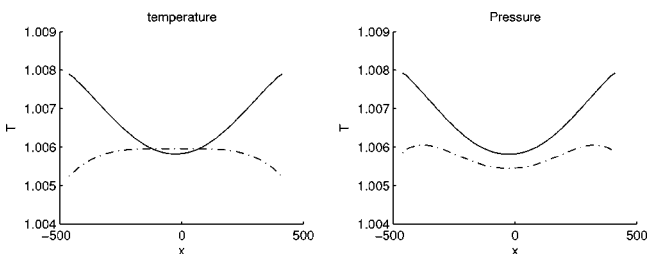


FIG. 3. Flow distribution in the cross-stream direction in the external force driven case at  $Kn=0.2$ . Dash-dotted lines: BGK Burnett solution, solid lines: BGK super-Burnett solution.

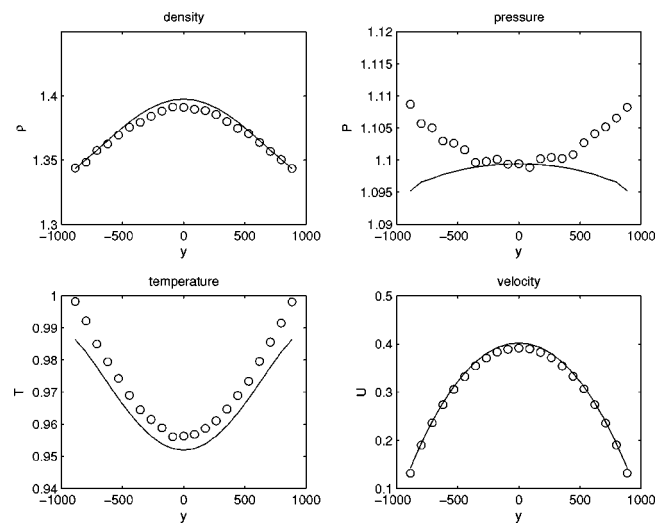


FIG. 4. Flow distribution in the cross-stream direction in the pressure driven case. Circles: DSMC results (Ref. 1), solid lines: BGK-Navier–Stokes solution.

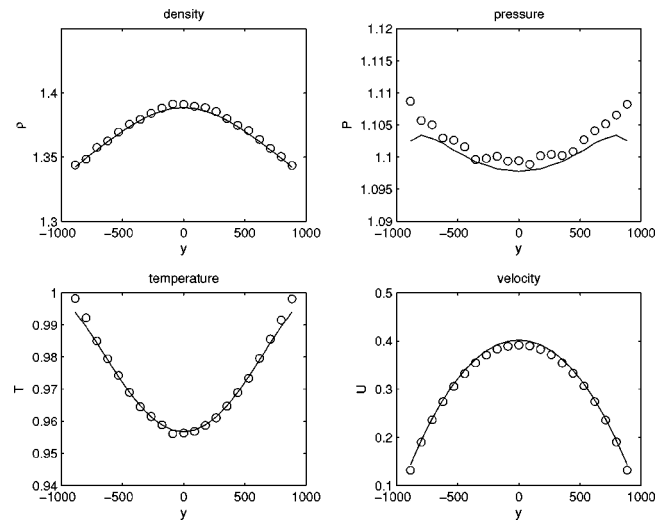


FIG. 5. Flow distribution in the cross-stream direction in the pressure driven case. Circles: DSMC results (Ref. 1), solid lines: BGK-Burnett solution.

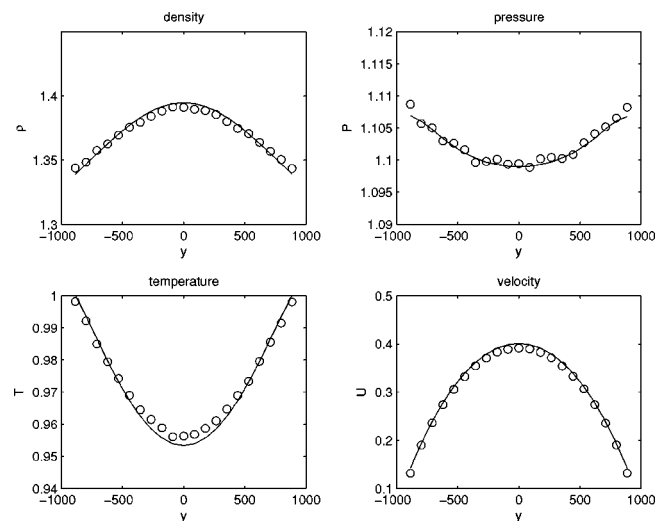


FIG. 6. Flow distribution in the cross-stream direction in the pressure driven case. Circles: DSMC results (Ref. 1), solid lines: BGK-super-Burnett solution.

Navier–Stokes solutions can be explained through the Burnett and super Burnett solutions. It confirms the analysis in Ref. 5 that the nonconstant pressure in the Poiseuille flow is coming from the Burnett order, and shows here that the temperature minimum phenomena is from the super-Burnett order. Also, the opposite curves in the pressure distribution between the Navier–Stokes and DSMC results in the pressure driven case can be resolved through both the Burnett and super-Burnett equations. Therefore, even in the slip flow regime, the development of Burnett and super Burnett flow solvers, such the current gas-kinetic BGK-super-Burnett method based on the evolution of the gas-distribution function and the method of Agarwal and Yun<sup>10</sup> based on macroscopic Burnett equations directly, may become necessary for the microflow simulation.

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