A Comprehensive Comparison of Higher-Order Moment Equations and DSMC for Force-Driven Poiseuille Gas Flow

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Abstract. The compressible Poiseuille gas flow within a channel driven by uniform body force emerges as a benchmark for testing the higher-order moment equations in the velocity shear dominated flow problems. The various solutions by NCCR theory, DSMC, and R-13 moment theory are compared comprehensively with emphasis on the physical behavior in phase space. Also, a simple method for the validation study of numerical solutions in high non-equilibrium flow problem is proposed. Using the new method, the accuracy of the numerical solutions in the force-driven Poiseuille gas flow, in particular, near the solid wall, is examined.

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INTRODUCTION

The compressible Poiseuille gas flow within a channel driven by uniform body force [1] emerges as a benchmark for testing the higher-order constitutive relations in the velocity shear dominated flow problems [2-4]. The mathematical problem involved is very simple owing to its pure one-dimensional nature, but it can bring out the essence of the non-classical constitutive relations in states removed from thermal equilibrium.

However, in contrast with the shock structure problem in the compression-dominated flow, the gas-surface molecular interaction near the solid wall becomes critical in the shear-dominated Poiseuille flow and, therefore, new theoretical and computational issues may become important. For example, most of the computational solutions will suffer numerical errors near the wall to some degree, since the theoretical models reflecting the true nature of gas-surface molecular interactions are not available.

In the present study, the various solutions by NCCR theory [2-4], DSMC calculation, and R-13 [5] are compared comprehensively with emphasis on their physical meaning and internal consistency. In addition, a simple method is proposed to examine the accuracy of the numerical solutions, in particular, near the solid wall.

DESCRIPTION OF THE FORCE-DRIVEN COMPRESSIBLE POISEUILLE GAS FLOW AND NCCR ANALYTICAL SOLUTION

The force-driven *compressible* Poiseuille flow is defined as a stationary flow in a rectangular channel under the action of a *uniform* external force parallel to the walls, as shown in Fig. 1. For a channel with high aspect ratio of length and height, the flow may be assumed fully developed and thus the associated mathematics will be greatly simplified. It is a simple, albeit very instructive, problem in the sense that it is purely one-dimensional but brings out the essence of the closure theory.

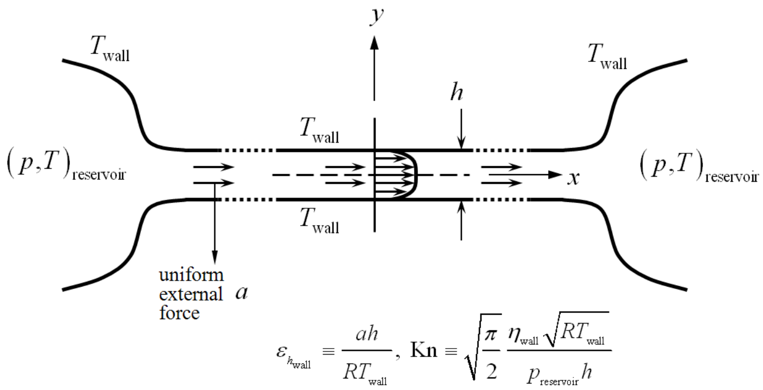

FIGURE 1. Description of the force-driven compressible Poiseuille gas flow between two pressure-regulated reservoirs.

In general, the analysis of this flow requires some level of numerical calculations when high degree of thermal non-equilibrium is considered: for example, DSMC and R-13 moment method. However, it was proven in previous works that a fully analytical approach is possible in the case of the NCCR (Nonlinear Coupled Constitutive Relation) theory. The analytical solutions of the following conservation laws [3],

$$\frac{d}{dy}\left[\Pi_{xy}, p+\Pi_{yy}, \Pi_{yz}, \Pi_{xy}u+Q_y\right]^T = \left[\rho a, 0, 0, \rho a u\right]^T, \tag{1}$$

can be summarized in a compact form as

$$\begin{aligned}
& p^*(S^*) = 1+\tan^2 S^*,\ \left[\Pi^*_{yy}(S^*)\right]_0 = -\frac{1}{N_\delta}\tan^2 S^*,\ \left[\Pi^*_{xy}(S^*)\right]_0 = \frac{1}{N_\delta}\sqrt{\frac{3}{2}}\tan S^*, \\
& \left[\Pi^*_{yy}\right]_0 = \left[\Pi^*_{zz}\right]_0 = -\frac{1}{2}\left[\Pi^*_{xx}\right]_0, \\
& u^*(S^*) = u^*(0)\left[1-4\alpha_V\left(\frac{\tan S^*}{2\tan S^*_{1/2}}\right)^2\right],\ \left[Q^*_y\right]_0 = \frac{1}{3}\Pr \mathrm{Ec} T_w^{*3}\frac{\varepsilon^2_{h_w}}{N^2_\delta}\left(\frac{\tan S^*}{2S^*_{1/2}}\right)^3 \\
& \left[Q^*_x\right]_0 = N_\delta\left[\left(1+\frac{1}{\Pr}\right)\left[\Pi^*_{xy}\right]_0\left[Q^*_y\right]_0 - \varepsilon_{h_w}\frac{T_r}{\Delta T}\frac{(\gamma-1)}{\gamma}\frac{T^*}{p^*}\left(2\left[\Pi^*_{yy}\right]_0 + N_\delta\left[\Pi^*_{xy}\right]_0^2\right)\right] \\
& T^*(S^*) = \sec^e S^*\left\{T^*(0) - \left[T^*(0) - \sec^{-e} S^*_{1/2}\left(\alpha_T T^*_w + (1-\alpha_T)T^*(0)\right)\right]\frac{F(S^*)}{F(S^*_{1/2})}\right\}
\end{aligned} \tag{2}$$

where an abbreviation $[A]_0 \equiv A - A(0)$ is introduced to represent the value of a quantity A measured from its value at the center, that is, $A(0)$, and,

$$\begin{aligned}
& S^* \equiv \sqrt{2/3}T^*_w \varepsilon_{h_w} s^*,\ \ Y^* \equiv \sqrt{2/3}T^*_w \varepsilon_{h_w} y^*,\ \ \alpha_{V,T} = \frac{1}{1+4\omega_{V,T}\mathrm{Kn}}, \\
& y^* = y/h,\ u^* = u/u_r,\ \ T^* = T/T_r,\ p^* = p/p(0),\ \Pi^* = \Pi/\left(\eta_w u_r/h\right),\ Q^* = Q/\left(k_w \Delta T/h\right),
\end{aligned}$$

$$u_r = \frac{2}{h}\int_0^{h/2} u dy,\ T_r = \frac{h/2}{\int_0^{h/2} T^{-1} dy},\ \ N_\delta = \sqrt{\frac{2\gamma}{\pi}}\ M\ \mathrm{Kn},$$

$$F\left(S^*\right) \equiv (4-e)\left[\frac{1}{(4-e)\cos^{4-e} s^*} - \frac{1}{(2-e)\cos^{2-e} s^*} - \left(\frac{1}{4-e} - \frac{1}{2-e}\right)\right],\ \ e = \frac{3(\gamma-1)}{2\gamma}.$$

Here $\omega_{V,T}$ denote velocity slip and temperature jump coefficients, respectively, which depend basically on the momentum and energy accommodation coefficients. The Maxwell molecules are assumed in the analytical study.

COMPREHENSIVE COMPARISION AND A NEW VERIFICATION SCHEME FOR HIGH NON-EQUILIBRIUM GAS FLOW

In order to compare the various solutions (compressible Navier-Stokes-Fourier, NCCR [3,4], DSMC, R-13 [5]) a case, ε_{h_w} =0.6 and Kn=0.1, is considered. The coefficient ω_V, ω_T in the slip model is assumed to be 1. Among various numerical solutions, the comprehensive DSMC result for a hard sphere gas and R-13 moment method result are chosen for the comparison study.

For the DSMC computation of Poiseuille flows, a one-dimensional system confined by two diffuse walls with T_w = 273 K is considered. The system is filled with *hard sphere* molecules with mass (m) of 5.0×10^{-26} kg and the diameter (d) with 4.0×10^{-10} m. The system size is 7.44×10^{-7} m and the number density (n_0) is 1.89×10^{25} m^{-3}. The corresponding mean free path (λ) is $\lambda = (2^{½}\pi n_0 d^2)^{-1} = 7.44 \times 10^{-8}$ m and the Knudsen number (Kn) is 0.1. In the present DSMC simulation, a single simulated particle represents 1.4×10^{15} molecules. To mimic the Poiseuille flow, each particle is accelerated by constant acceleration of $1.6 \times 10^{-4} \times (2k_B T/md)$ m/s^2. The computational domain is divided by 50 uniform cells and each cell consists of 10 sub-cells for better accuracy. About 10,000 particles are introduced into the system. During a time-step of DSMC simulation Δt, the particles travel (advection stage) and then, the collisions are tested for all the possible pairs of particles in a computing cell using acceptance-rejection procedure (collision stage). The particles move in channel direction only, while the velocities are computed for all three-directions. Once the system reaches steady state, another 10,000 steps proceed for sampling data, which produce about 60,000,000 collisions.

First, the well-known abnormal properties (non-uniform pressure distribution and central temperature minimum) in the force-driven compressible Poiseuille flow problem are compared in Fig. 2. The NCCR solution was shown to predict the temperature minimum near the center in the force-driven Poiseuille flow. When the analytical temperature solution (2) is examined, it is obvious that the central temperature minimum is caused by the factor $\sec^e S^*$. Note that the factor can be expanded as $\sec^e S^* = 1 + (e/2) S^{*^2} + O(S^{*4})$. On the other hand, the positive monotonic function $F(S^*)$ plays a role similar to the quartic function y^{*^4} in the case of the Navier-Stokes-Fourier theory, since it can be expanded as $F\left(S^*\right) = (1-e/4) S^{*4} + O(S^{*6})$.

A close examination of the analytical solution of the NCCR theory summarized in the previous section reveals the existence of a kinematic constraint on viscous shear and normal stresses, implying their inter-dependence. It will be very instructive to compare various solutions in phase diagram of stress, as shown in Fig. 3. It can be observed that the NCCR theory is in qualitative agreement with the DSMC prediction, even though some mismatch is found near the solid wall. A definite explanation for this disagreement is not yet available and the further study is needed to resolve the issue.

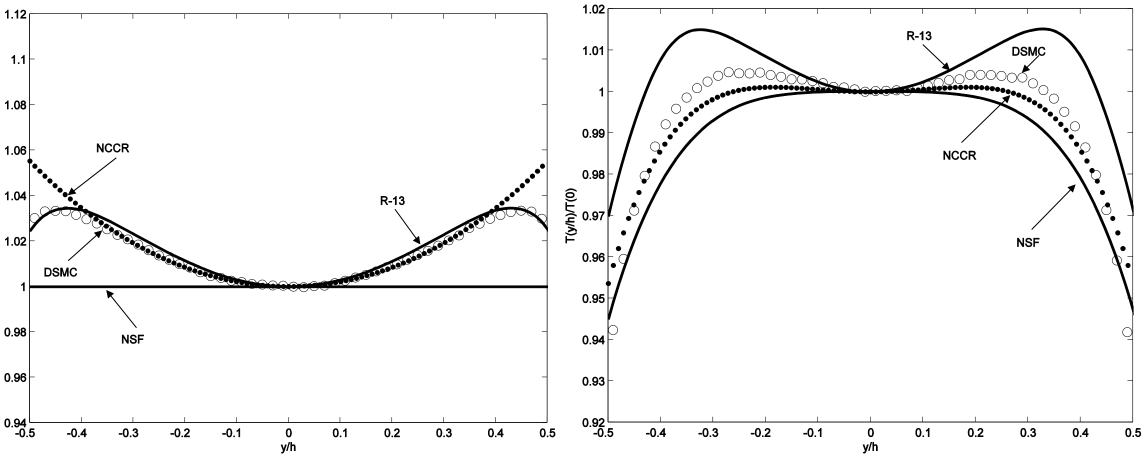

FIGURE 2. Comparison of the various solutions in the force-driven compressible Poiseuille gas flow (Kn=0.1, ε_{h_w} =0.6) : (a) pressure $p(y^*)/p(0)$ (left), (b) temperature $T(y^*)/T(0)$ (right).

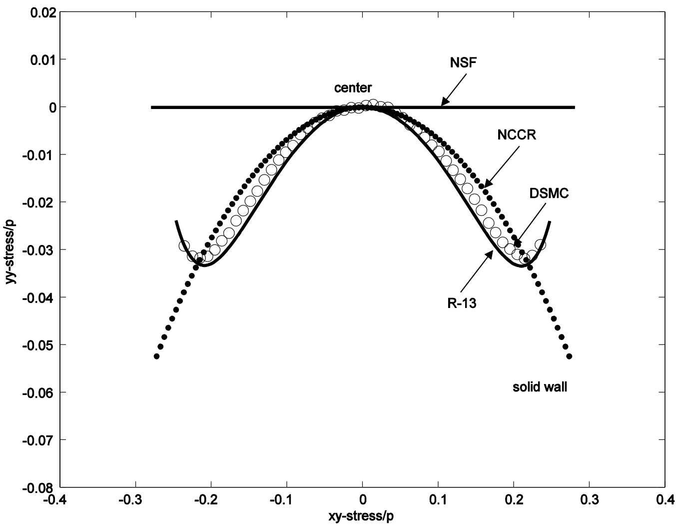

FIGURE 3. Comparison of the solutions in phase diagram of stress ($\left[\Pi_{xy}\right]_0/p$ vs $\left[\Pi_{yy}\right]_0/p$) in the force-driven compressible Poiseuille gas flow (Kn=0.1, ε_{h_w} =0.6).

It is well known that the validation of numerical solutions for high non-equilibrium flow such as rarefied and micro- and nano-scale gases is extremely difficulty due to the lack of experimental data. In particular, flows involving with the solid surface are considered most challenging because the velocity slip and temperature jump boundary conditions make the validation study even worse. However, there can be a self-consistent verification method if one recalls the fact that the conservation laws must be satisfied irrespective of computational models. Furthermore, such scheme can be easily applied in the case of the pure one-dimensional problem. Here such a validation study on DSMC solutions is conducted by checking the *relative* internal error of its solutions; for example, the x -momentum equation of the conservation laws (1),

$$\text{error}_{x\text{-momentum}} \equiv \frac{\Pi_{xy}(y) - \int_0^y \rho(y) a dy}{\rho(0) a h}, \tag{3}$$

or

$$\text{error}_{x\text{-momentum}} \equiv \frac{T(0)}{\varepsilon_{h_w} T_w} \frac{\Pi_{xy}(y^*)}{p(0)} - \int_0^{y^*} \frac{\rho(y^*)}{\rho(0)} dy^* . \qquad (4)$$

The computational error of DSMC is plotted in Fig. 4. In the case of NCCR theory, there exists no error owing to the analytical approach taken throughout. It can be observed that the relative error of DSMC increases from the center to the solid wall and reaches a maximum 1.4% near the wall.

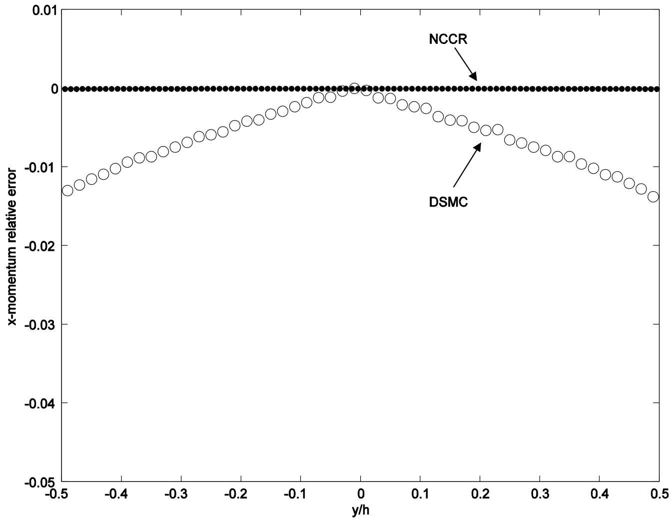

FIGURE 4. Distribution of errors in the conservation law of x -momentum across the channel in the force-driven compressible Poiseuille gas flow (Kn=0.1, ε_{h_w} =0.6).

CONCLUSIONS

A comprehensive comparison of various solutions for the force-driven Poiseuille gas flow is presented. All the solutions are in qualitative agreement throughout the domain, even though some mismatch is found near the solid wall. A simple method for the validation of numerical solutions in high non-equilibrium flow problem is proposed and applied to the force-driven Poiseuille gas flow. Non-negligible relative error in DSMC data is found near the solid wall.

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