

Scaling Issues for Calculations of Low-Velocity Gaseous Microflows

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ABSTRACT

Gaseous flows in microfluidic devices are often characterized by relatively high Knudsen numbers, Kn . For such flows, the continuum approximation is not valid, and Direct Simulation Monte Carlo (DSMC) is an appropriate solution method. However, for slow flows, where the fluid velocity is much smaller than the mean molecular velocity, the statistical fluctuations in the solution cause the features of the flow to be lost in the noise. In this paper, we evaluate a method for solving low-velocity microflows by scaling the temperature of the fluid such that the molecular thermal velocity is on the same order of magnitude as the fluid velocity. We present an analysis of this scaling method, and show how modification of the fluid temperature affects the collision dynamics.

Keywords: Direct Simulation Monte Carlo, microflows, high Knudsen number flows

INTRODUCTION

Many practical MEMS devices involve gas flows in micron-sized systems at very low velocities. These are characterized by relatively high Knudsen numbers, $Kn = \lambda/L$, where λ is the mean free path and L is a characteristic length. For a gas in a microdevice at 1 atm and 298 K, $Kn \sim 0.15-0.20$, which means that the continuum approximation does not apply. One possible method for computing the properties of such flows is DSMC, which is a statistical method in which the motion and interactions of a number of simulated particles are used to modify their positions and velocities [1,2]. However, for very low-velocity flows, DSMC is not practical because it requires too many timesteps for the particles to pass through the entire computational domain and too many particles.

An additional problem occurs when the flow velocity, V_f , is much smaller than the mean molecular thermal velocity, V_t . For a gas at 1 atm and 298 K, $V_t \sim 100,000$ cm/s. If $V_f = 20$ cm/s, the statistical noise is 10^4 greater than the solution and features of the flow are completely lost in the noise. In principle, the correct

result should emerge as the ensemble or time average converges, because the statistical fluctuations decrease with the number of samples. However, too many timesteps ($\sim 10^8$) are required to resolve such a low-velocity flow. In this paper, we evaluate a method for solving low-velocity microflows by scaling the temperature of the fluid, such that the V_t is on the same order of magnitude as V_f , thereby reducing the statistical noise.

NUMERICAL METHOD

The core of the DSMC algorithm consists of four primary processes: move the particles, index and cross-reference the particles, simulate collisions, and sample the flow field. These procedures are uncoupled during each timestep. Of primary importance is the selection of a timestep that is on the order of the local mean collision time and cell size that is on the order of the local mean free path. The first process, moving simulated molecules, enforces the boundary conditions and samples macroscopic properties along solid surfaces. The second process involves indexing and tracking the particles. The next step is simulating collisions between randomly selected pairs of molecules within each cell. The currently preferred collision model is the no-time-counter technique, used in conjunction with the sub-cell technique [1]. The sub-cell method calculates local collision rates based on the individual cells, but restricts possible collision pairs to sub-cells. This procedure improves accuracy by ensuring that collisions occur only between near neighbors. The final process is sampling the macroscopic flow properties. The properties of molecules in a particular cell are used to calculate macroscopic quantities at the geometric center of that cell.

RESULTS AND DISCUSSION

We present a series of calculations designed to evaluate whether a scaled solution can be used to deal with the problem of statistical noise. The approach is to scale the temperature so that V_t is the same order of magnitude as V_f . We test this scaling approach on a problem for

which we can compute the “correct” solution, and then compare it with a scaled solution. The tests consist of a series of two-dimensional DSMC calculations for helium in a $1 \times 12 \mu\text{m}^2$ channel at 60,000 cm/s. The correct solution is the DSMC calculation at 298 K, while the scaled solution is at 165K. Figure 1 shows that the shape of the temperature profiles are almost identical for the two cases, and only differ by the constant scaling factor. Although the shape of the pressure profiles are similar, the difference in pressure is greater at the inflow than at the outflow boundary. Similar differences appear in the density profile, however, the velocity profiles for the two cases are essentially identical. As discussed further below, changing the fluid temperature does affect the collision dynamics, and the differences between the correct and scaled solutions are attributed to this phenomenon.

As most MEMS applications involve slow flows, simulations at even lower velocities were conducted. A test case at $V_f=200$ cm/s, 1 atm and 298 K was attempted, but the solution was still dominated by statistical noise even after 15,000 timesteps. By significantly reducing the temperature, such that V_i was on the same order of magnitude as V_f , a converged calculation was achieved within 2000 timesteps. Figure 2 shows a comparison of the velocity profile for the scaled and unscaled calculations, and illustrates the statistical noise problem for the unscaled case.

This scaling technique alters the fluid temperature, and therefore has an effect on the collision dynamics. Figures 3-a, -b, and -c show the relationship between the relative velocity (c_r) between colliding particles, the collision cross section (σ), and the average product of σc_r with temperature, for the 200 cm/s unscaled test case discussed above. Data are presented for both Hard Sphere (HS) and Variable Hard Sphere (VHS) particles. The HS model is a simplified molecular model in which σ is constant, while the VHS molecular model is more realistic and includes the dependence of σ on c_r . The average c_r is a function of temperature for both HS and VHS particles, as shown in the overlapping curves of Fig 3-a. As shown in Fig. 3-b, σ is constant for HS particles, but is temperature-dependent for the more realistic VHS molecular model. That is, for a VHS particle, σ can be expressed as a function of c_r , which is a function of temperature:

$$\sigma = \frac{\pi d_{ref}^2}{4} \sqrt{\frac{2kT_{ref}}{m_r c_r^2}}^{\omega-1/2} \quad (1)$$

where d_{ref} and T_{ref} are a fixed reference diameter and temperature, respectively, m_r is the reduced mass, and

is the temperature-viscosity coefficient. Since $\omega = 1/2$ for HS particles, σ is a constant and is independent of c_r . For VHS particles, $1/2 < \omega < 1$, and therefore, as the fluid temperature decreases, c_r decreases sharply (Fig 3-a), and σ increases (Eq. 1), as shown in Fig. 3-b. Therefore, the average product of σc_r decreases with decreasing temperature (because c_r decreases sharply with decreasing temperature), as shown in Fig 3-c. Since this product is used in the calculation of collision probabilities between two particles, it is important to quantify the effect of temperature scaling on the collision dynamics. Despite these effects, temperature scaling provides a more accurate solution than solving high Kn flows with the Navier-Stokes equations alone.

Another potential method to reducing statistical noise is to combine a DSMC and Navier-Stokes (NS) solution. By using both methods interactively, the output from one method can provide the input conditions for the other method. In this sense, the DSMC calculation may be viewed as providing the physically correct boundary conditions and transport coefficients in high-Kn flow regimes to the NS computation. Previous work on a high-speed microchannel flow problem [3] showed that using NS as a filter for the DSMC calculation could eliminate some of the noise and reduce the computational time. However, the filtering could not be applied until a near-steady solution had been attained. Similar results were obtained for this study of low-velocity flows. That is, for the 200 cm/s case, the DSMC solution, even after 15000 timesteps, was still too noisy and not sufficiently converged to achieve any benefit from the NS filter.

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ACKNOWLEDGEMENTS

This project is supported by the DARPA Design for Mixed Technology Integration Program. Computing resources were supplied by the DoD High Performance Computing Modernization Program. The authors gratefully acknowledge helpful DSMC discussions with Drs. Choong Oh, Bohdan Cybyk and David Fyfe.

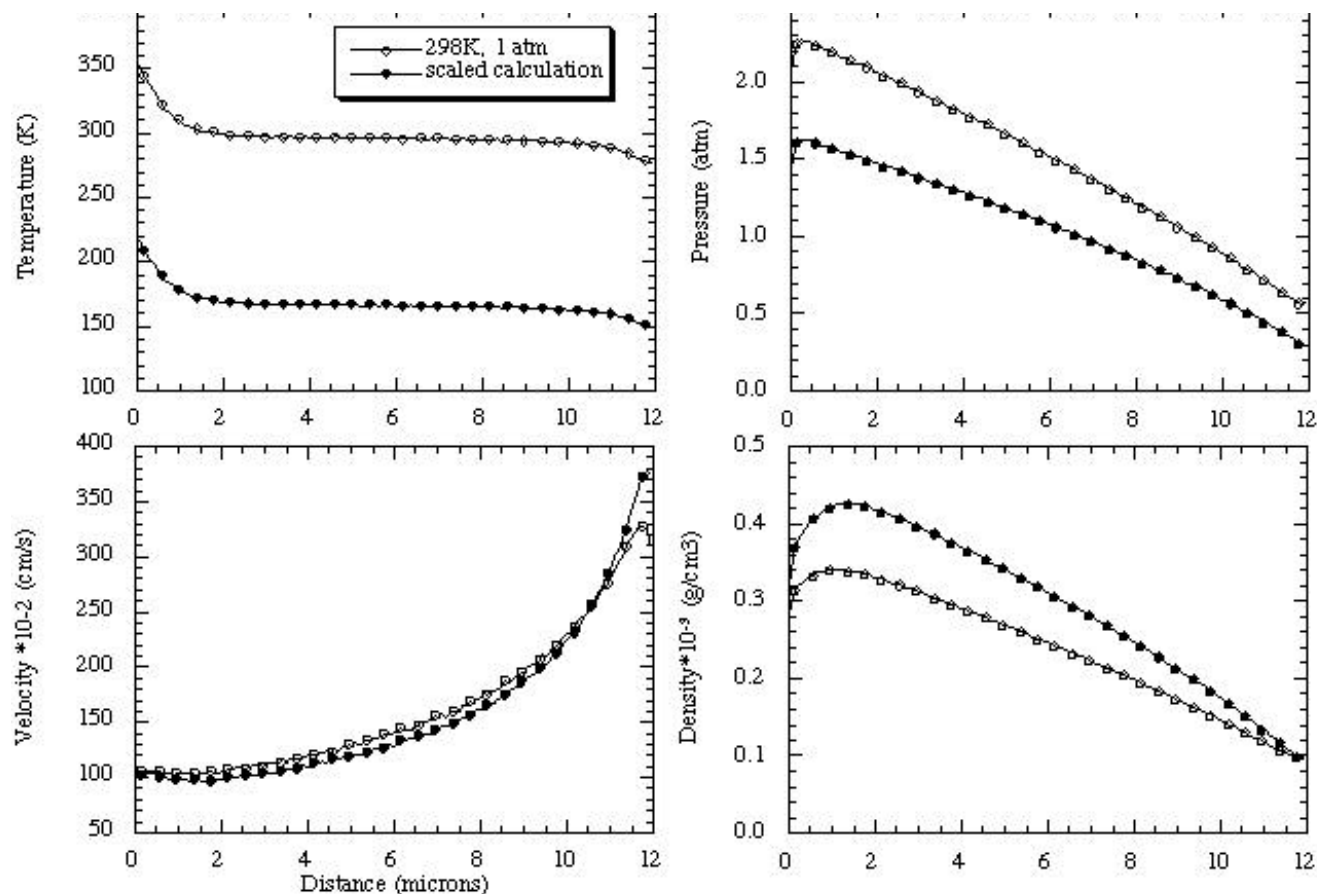


Figure 1. Preliminary tests of the temperature scaling method. Open circles correspond to the correct calculation at 60,000 cm/s, 298 K, and 1 atm. The scaled calculation was done at the same velocity, but at reduced temperature and pressure, at 165 K, 0.6 atm. The plotted quantities are values along the longitudinal channel centerline.

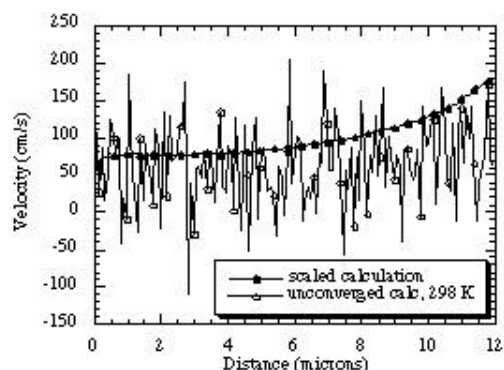


Figure 2. Comparison of the velocity profile (in the longitudinal direction) for the scaled and unscaled calculations. The data are shown after 2000 timesteps for the scaled, and after 15000 timesteps for the unscaled calculations. Statistical noise overwhelms the solution for the unscaled case.

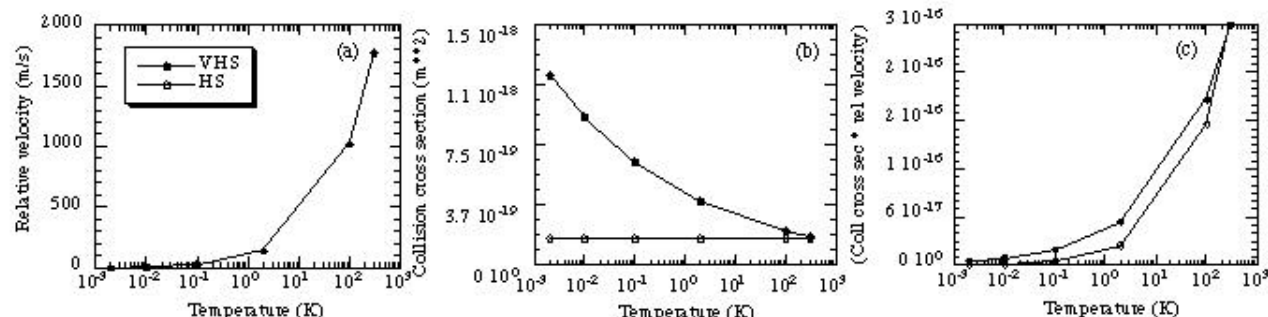


Figure 3. The relationship between temperature and (a) average relative velocity between colliding particles, (b) collision cross section, and (c) the average product of the collision cross section and relative velocity. The relative velocity curves for HS and VHS particles overlap in Fig. 3-a