Failure analysis of the molecular block model for the direct simulation Monte Carlo method

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The present Brief Communication analyzed and demonstrated the failures of the molecular block (MB) model for the direct simulation Monte Carlo (DSMC) method. In the MB model, the gas viscosity and Knudsen number remained the same but the Mach number increased with the MB factor α. Therefore, the flow predicted by the MB model failed to agree with the original flow. Micro Couette flows and microchannel flows were simulated to demonstrate this point. Significant differences were found between results from the MB model and the original DSMC method. When α was large enough so that the Mach number in the MB model exceeded unity, a shock wave appeared in the channel, when there were no shocks in the original subsonic flow. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1707043]

Many researchers have applied Bird's direct simulation Monte Carlo (DSMC) method[1] to predict the high-speed gas flow and heat transfer in microchannels.[2,3] However, supersonic gas flow seldom occurs in microchannels. Most of gas flows in microelectromechanical systems (MEMS) devices are subsonic, on the order of 10 $m \cdot s^{-1}$ or less. Thus, the small macroscopic velocity can be obscured by the large molecular thermal movement velocities, which are over 300 $m \cdot s^{-1}$ at ordinary temperatures. Therefore, large statistical errors are a serious problem faced by the DSMC method for simulation of low-speed flows. In theory, the statistical error, which is inversely proportional to the square root of the sample size, will decrease to zero with an infinite sample size. However, in fact the expected trend is limited by one fact that the random process generated by a computer simulation is a quasirandom process but not a real one. As a result, the DSMC method is not just limited by the high computational cost but also by the unrealistic belief that the statistical error in the DSMC method will become satisfactorily small by increasing the sample size.[4]

Improvements have been proposed to decrease the statistical error of DSMC. A method called DSMC-IP (Information Preservation) was presented by Fan and Shen,[5] and then developed by Cai *et al.*[6,7] The IP method has successfully simulated low-speed gas flow in microchannels; however, at the cost of increased complexity and additional memory and computation costs. Pan *et al.*[4] investigated the features of the DSMC statistical errors and found that the magnitude of the statistical error depends on the gas temperature and gas type: lower temperatures and/or larger molecular masses result in smaller statistical errors. Two modified DSMC methods were then proposed. The first was based on the dependence of the statistical error on the temperature, but could not calculate the temperature field and could not be easily expanded to two or three dimensions. The second was based on the dependence of the statistical error on the gas molecular mass.[8] In this method, molecular blocks replaced the original molecules, so the method was named MB-DSMC. The principle of the MB-DSMC method is simple with little complexity or increased computational cost. If the effectiveness of the method could be proved, the method would revolutionize DSMC simulations of microgas flows. Unfortunately, this method fails in the simulations. Recently, Hadjiconstantinou *et al.* have found that there is no way to reduce the statistical errors in the measurement of flow velocity without changing the Mach number.[9] The present Brief Communication will analyze the failures of the MB-DSMC method. Both theoretical analysis and simulated results show the failures of the MB-DSMC calculations; therefore, much work is needed to improve the method.

The basic assumption of the MB model is based on the dependence of the statistical error on the gas molecular mass. From the Maxwellian distribution of gas molecules at an equilibrium state, the random thermal velocity is proportional to the most probable molecular thermal velocity, i.e.,

$$V' \propto \sqrt{\frac{2kT}{m}}, \tag{1}$$

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where k is the Boltzmann constant, T is the macroscopic temperature, and m is the molecular mass. Since the statistical error of the stream velocity is a nonzero mean value of the random thermal velocity, the statistical velocity error, δV_0, is also proportional to the most probable molecular thermal velocity for a given sample size

$$\delta V_0 \propto \sqrt{\frac{2kT}{m}}. \tag{2}$$

Equation (2) indicates that if the molecular mass increases α times, the statistical velocity error will contract $\sqrt{\alpha}$ times for the given temperature and sample size. So the molecular block model algorithm can be described by the following sets of equations:

$$m_b = \alpha m, \tag{3}$$

$$d_{b,\mathrm{ref}} = \alpha^{1/4} d_{\mathrm{ref}}, \tag{4}$$

$$n_b = \alpha^{-1/2} n, \tag{5}$$

$$\Gamma_b = \alpha^{1/2} \Gamma, \tag{6}$$

where the subscript b denotes quantities of the MB model, d_{ref} the reference diameter, n the number density, and Γ the collision rate. Equations (4) and (5) were derived to maintain the values of the mean free path, λ, and the macroscopic viscosity, μ.

The macroscopic gas properties can be calculated by

$$\rho = \frac{n_b m_b}{\sqrt{\alpha}} = \frac{\rho_b}{\sqrt{\alpha}}, \tag{7}$$

$$V = V_b, \tag{8}$$

$$T = \frac{m_b}{3k}\overline{(V_b')^2} = T_b, \tag{9}$$

$$P = \sqrt{\alpha} n_b m_b \overline{V_b' V_b'} = \sqrt{\alpha} P_b. \tag{10}$$

The molecular block model algorithm is then described by Eqs. (3)–(10). Pan *et al.*[8] simulated micro Couette flow and micro Poiseuille flow using the modified MB-DSMC codes. They also reported that the velocity precision was not significantly improved for α greater than 1000. They suggested a good choice for α to be around 100, but no reason was given.

The derivation of the MB model seems to be reasonable for the original DSMC method. However, the model fails in the simulations. In the following the failure is analyzed.

From the kinetic theory, the Knudsen number is defined as

$$\mathrm{Kn} = \frac{\lambda}{l} = \frac{\mu\sqrt{m\pi}}{\rho l \sqrt{2kT}}, \tag{11}$$

where λ is the gas mean free path and l is the characteristic length. The Knudsen number for the MB model is

$$\mathrm{Kn}_b = \frac{\mu_b \sqrt{m_b \pi}}{\rho_b l \sqrt{2kT_b}} = \frac{\mu\sqrt{\alpha m \pi}}{\sqrt{\alpha}\rho l \sqrt{2kT}} = \mathrm{Kn}, \tag{12}$$

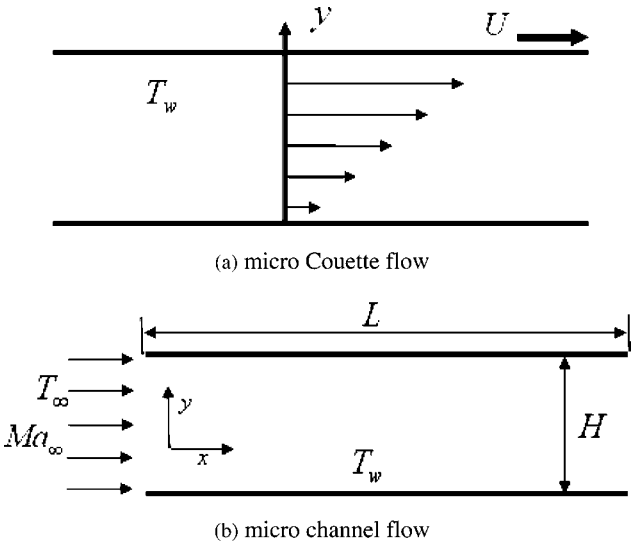

FIG. 1. Geometries and boundary conditions for the simulated microflows. (a) Micro Couette flow; (b) microchannel flow.

where the gas viscosity μ is assumed dependent only upon the temperature.

The sound speed propagating in a gas is well known to be a function of the gas temperature and the gas type

$$a = \sqrt{\gamma R T} = \sqrt{\gamma k T/m}, \tag{13}$$

where a is the local sound speed, γ is the specific heat ratio, R is the gas constant, T is the local temperature, k is the Boltzmann constant, and m is the molecular mass of the gas.

According to Eqs. (3) and (9) of the molecular block model, the sound speed is

$$a_b = \sqrt{\gamma k T_b/m_b} = a/\sqrt{\alpha}. \tag{14}$$

Combining Eq. (14) with Eq. (8) gives the Mach number in the MB model

$$\mathrm{Ma}_b = \sqrt{\alpha}\,\mathrm{Ma}. \tag{15}$$

Equations (12) and (15) show that though the Knudsen number remains, the Mach number in an MB calculation differs from the original gas when α is not equal to unity. However, two flows will be similar only when the dimensionless similarity criterions, which are the Reynolds number, the Mach number and the Knudsen number, are equal.[10,11] Therefore, the flow state in the MB model really changes from the original flow in theory.

Equation (15) also indicates that the Mach number in the MB model is $\sqrt{\alpha}$ times that of the real Mach number. Therefore, when the value of α is too large, the Mach number of the MB model could exceed unity, and a shock wave would appear when no such shock wave occurred in the original (subsonic) flow.

Two flow cases were simulated to demonstrate the failure of the MB model. The standard codes from Bird[2] were developed. Micro Couette flows and microchannel flows were analyzed with different α values. The physical geometries and boundary conditions are shown in Fig. 1. Nitrogen gas flows between the planes with the properties from Bird's book[2] listed in Table I. The variable hard sphere (VHS) model and the diffusive wall boundary condition were used

TABLE I. Properties of nitrogen gas.[a]

m ($\times 10^{-26}$ kg)	ζ	d_{ref} ($\times 10^{-10}$ m)	T_{ref} (K)	ω	γ
4.65	2	4.17	273	0.74	1.4

[a]m is the gas molecular mass, ζ is the internal energy degrees of freedom, d_{ref} is the reference molecular diameter, T_{ref} is the reference temperature, ω is the viscosity–temperature index, and γ is the specific heat ratio.

for the collision processes. The Larsen–Borgnakke model with discrete rotational energies was used to model the energy exchange between the translational and internal modes.

For the one-dimensional microplane Couette flow [Fig. 1(a)], the distance between the two planes was 0.1 μm with the height divided into 100 cells. Each cell had more than 20 simulated particles. The initial molecular number density is 2.68×10^{25}, so the Knudsen number is 0.48. Both the initial gas temperature and the wall temperature were 273 K. The upper plane moved at a speed of $U=2\ \mathrm{m\cdot s^{-1}}$. The α values ranged from 1 to 100.

The simulated nondimensional x-velocity distributions are shown in Fig. 2. Although the sample size for each case is 2×10^7, the relative fluctuations are distinct due to the quite low Mach number. However, it is clear that the x-velocity distributions vary with the values of α. When α is unity, the MB-DSMC is equivalent to the original DSMC. When α is larger than unity, the MB model results differ greatly from the original DSMC results. For large values of α (such as $\alpha>20$), the velocity distributions are close to each other for different α. Pan *et al.*[8] compared the original DSMC results for the Couette flow only with $\alpha\geqslant25$ in small sample sizes, which may be why they did not find the differences between the original DSMC and the MB model.

The subsonic channel internal flows are considered. Equation (15) shows that the Mach number in the MB model is $\sqrt{\alpha}$ times the original Mach number. As a result, when α is large enough so that the Mach number in the MB model exceeds unity, a shock wave will appear, when no such shock wave was apparent in the original (subsonic) flow.

The physical geometry and the boundary conditions for the flow are shown in Fig. 1(b). The channel was 4 μm long and 1 μm high. The freestream Mach number Ma_∞ was 0.283. Both the incoming gas and the wall temperatures were 300 K. The working fluid was nitrogen gas. The initial Knudsen number was specified at 0.1. The grid included 60×30

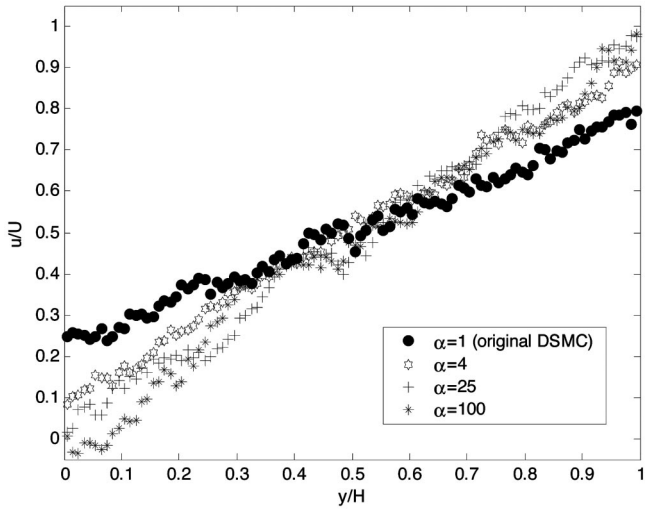

FIG. 2. Comparisons of nondimensional x-velocity distributions for nitrogen gas micro Couette flow at Kn=0.48 and $U=2\ \mathrm{m\cdot s^{-1}}$.

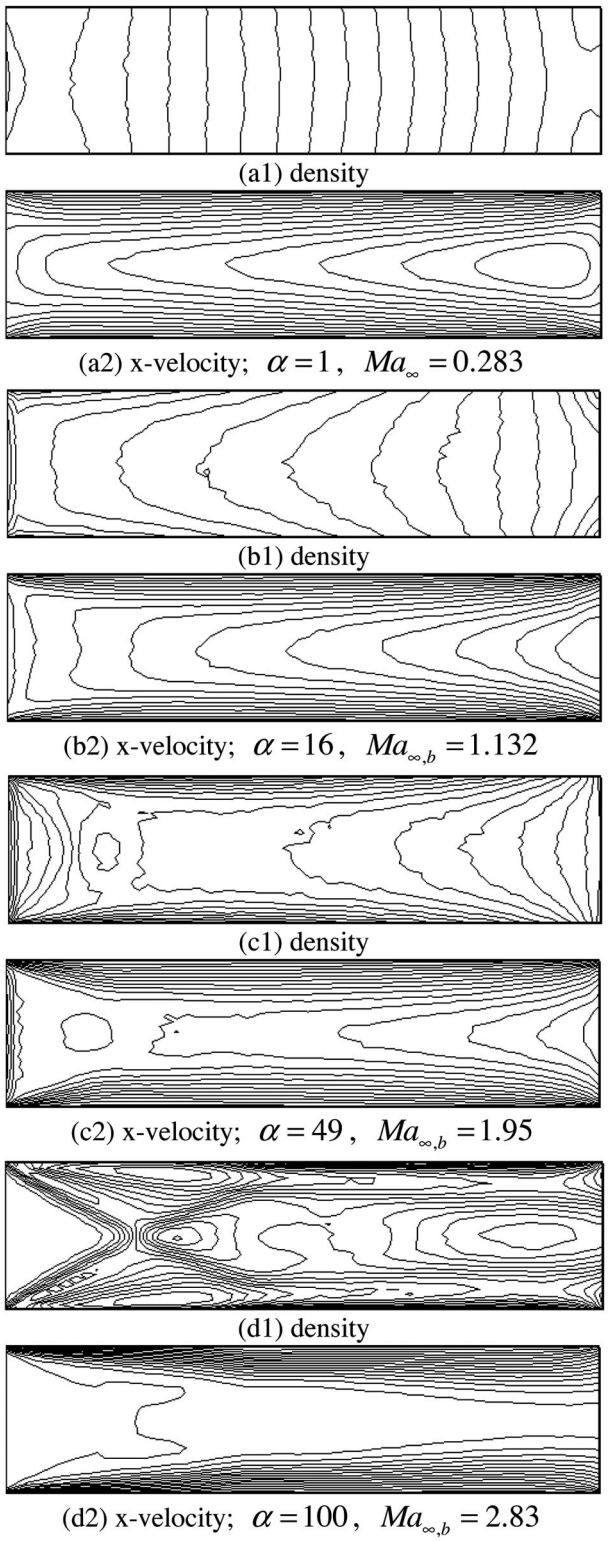

FIG. 3. Simulation results for internal flow at different values of α, $\mathrm{Ma}_\infty=0.283$, Kn=0.1. (a) Density and x-velocity contours for $\alpha=1$; (b) density and x-velocity contours for $\alpha=16$; (c) density and x-velocity contours for $\alpha=49$; (d) density and x-velocity contours for $\alpha=100$.

uniform rectangular cells with 2×2 subcells in each cell. The values of α varied from 1 to 100. The calculated density and x-velocity contours are shown in Fig. 3. For the subsonic channel flow at $Ma_\infty<0.3$ shown in Fig. 3(a), the density distribution along the channel obtained from the original DSMC is nearly linear, and the density across the channel is nearly uniform. The x-velocity along the channel midline increases monotonously. For $\alpha=16$, the freestream Mach number in the MB model should be a little higher than 1.0 according to Eq. (15), so the internal flow is then in high Mach number. The density distribution along the channel is no longer linear, and the density in each section is not uniform, as shown in Fig. 3(b). When α is larger, a shock wave will appear, even though there was no such shock wave in the real flow. A weak shock wave develops for $\alpha=49$ ($Ma_b=1.95$) in Fig. 3(c) and a strong shock wave develops for $\alpha=100$ ($Ma_b=2.83$) in Fig. 3(d). The density and x-velocity variations are no longer monotonous along the channel but vary rapidly in each section. The results indicate the failure of the MB model.

In summary, the present paper analyzed and demonstrated the failures of the Molecular Block model. The Knudsen number in the MB model remains but the Mach number of the MB model is $\sqrt{\alpha}$ times the Mach number of original DSMC. Therefore, the flow state of the MB model differs from that of the original DSMC. When the value of α is so large that the Mach number of the MB model exceeds unity, a shock wave appears, when no such shock wave occurred in the original flow.

Appendix: Implementation of the molecular block model. The standard DSMC codes were obtained from Bird's web site,[12] and the code for the Couette flow is DSMC1.FOR.

In the subroutine DATA1, the molecular mass [SP(5,1)], diameter [SP(1,1)] and the number density [FND] were transferred to the value in MB model based on Eqs. (3)–(5). The time step is determined by

$$\Delta t=\frac{1}{4}\frac{\Delta x}{\sqrt{2kT/m_b}}. \tag{A1}$$

For the MB-DSMC method, the probable collision pairs in the cell in one time step are obtained by[8]

$$S_p=\frac{\sqrt{\alpha}}{2}\overline{N_b}N_bF_{Nb}(\sigma_{T,b}c_{r,b})_{\max}\frac{\Delta t}{V_c}. \tag{A2}$$

In the subroutine COLLMR, the value of ASEL in the MB model is $\sqrt{\alpha}$ times of the original value based on Eq. (A2).

Before outputting the sampled flow characteristics, the values in the MB model should be reverted to original values based on Eqs. (7)–(10).

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