Direct Numerical Simulation of A Forced Micro Couette Flow using DSMC

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Abstract. The direct simulation Monte Carlo (DSMC) method is used in a time-dependent manner to simulate three-dimensional micro Couette flows. An artificial forcing that mimics the centrifugal force in the Taylor problem has been applied to the flow. The sampled behaviors of the resulting flow, including the averaged properties and disturbances, are studied. The computations have been performed using a parallel computer cluster. The results presented include those with various channel heights, plate speeds, and the forcing level. These changes also result in changes in the flow Reynolds number and Knudsen number. Spatially coherent flow patterns can be identified in the averaged flow and the disturbance flow fields. The results indicate that the discrete approach can capture unsteady, three-dimensional vortical flow structures. In cases with strong forcing, the disturbance energy spectra show significant content above statistical scatter.

INTRODUCTION

Microelectromechanical systems (MEMS) technologies have had significant impacts in different areas such as biosciences, computer sciences, and telecommunication. Many of these realized devices use fluid as a working media and their designs have often been guided by correlations derived from the fluid flow behavior observed at macroscales. With the increasing demand for higher system complexity and performance, it is important to develop a better understanding of the fluid flow characteristics at the microscale.

Many recent experiments in fluidic microchannels have reported significant differences in the heat and momentum transfer coefficients compared with those at the macroscale. For example, while the friction factor varies inversely with the Reynolds number when the Reynolds number is small, the proportionality constant does not agree with the conventional correlation. The friction factors are also found to diverge from this inverse proportionality, which at macroscale indicates a change of flow characteristics from that of a laminar flow to a turbulent flow, at smaller Reynolds numbers than those commonly observed in the corresponding large channels. This early change of flow characteristics has been attributed to the effects of, for instances, gas rarefaction and other surface mechanisms, the large change of the flow Reynolds number along the microchannels, and the likely experimental uncertainties in microscale measurements. Advanced measurement techniques such as molecular tagging can produce more detailed quantitative data for microflows, which may eventually lead to a better understanding of the apparent microflow transition. In this paper, results obtained in recent micro Couette gas flow simulations will be presented. The DSMC method pioneered by Bird [1] is used. With an artificially applied, adjustable forcing, the flow model is used to study capturing the unsteady, three-dimensional flow disturbances in microflows.

The DSMC method has been applied to many different fluid dynamics problems. It has been widely used in the simulations of rarefied gas flow. The method has also recently been applied to calculate the fluid flow and heat transfer behaviors of microchannels.[2,3] DSMC has been employed to study the low-density limits of a number of flow instabilities. The centrifugal instabilities in Taylor-Couette flows have received the most attention.[4,5] The formation of Taylor vortices were clearly demonstrated for a range of Knudsen number in these two-dimensional

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(axisymmetric) flow computations. The convective instability associated with the Rayleigh-Bénard cells has also been studied.[6]

DSMC applies a molecular description of gases. Gases are recognized as a myriad of discrete molecules and the positions, velocities, and states of molecules are recorded at all time. The computational molecules are allowed to move and collide in the physical space. Macroscale flow properties can be obtained by sample averaging. For gas flows in microscaled geometry, the Knudsen number based on the characteristic size of the geometry can be large. The applicability of the linear constitutive relations in the Navier-Stokes equations, which are used in the direct numerical simulations of macroscale flows, becomes questionable due to the large flow gradients. In fact, when one considers the local, smaller scale flow events, the value of the local Knudsen number can further increase. The DSMC method is based on first principles and is not limited to small Knudsen number. DSMC is appropriate for the direct numerical simulations of such microflows. As the DSMC method uses a molecular description of gases, there have been concerns[7] whether DSMC is capable of resolving vortical fluid motions due to the lack of an exact conservation of angular momentum in collisions. Results obtained by Nanbu et al.[8] shows that as long as the cell size is sufficiently small, the total angular momentum is nearly conserved. Bird[9] has also shown that the non-conservation of the angular momentum has no significant effects on the DSMC solutions. The gas flows in complex microfluidic systems are expected to be three-dimensional and unsteady. As an eligible direct numerical simulations tool for microflows, it is then important for DSMC to be able to resolve also the unsteady flow disturbances with three-dimensional structures. DSMC allows for a direct physical simulation of gas flows. The minimum level of physical modeling is needed at the level of molecular models that have been used in kinetic theory of gases. However, a large number of particles are required in a DSMC simulation to reduce the inherent statistical scatter. The computer resource needed to perform three-dimensional flow simulations can be significant, which appears to be a major limiting factor for performing many necessary simulations to capture three-dimensional physical flow disturbances. Many efforts have been made to take advantage of the advent of parallel computing to reduce the time required for DSMC simulations. The simulations presented here have been performed by the use of a parallel DSMC algorithm[10] and a parallel computer cluster, CEPCOM, in the CFD Lab. at Western Michigan University.

In this paper, results of three-dimensional time-dependent microflow simulations using parallel DSMC computation will be presented. The flow geometry considered is shown in Figure 1. The flow develops between two diffuse walls in the y-direction, the top wall moves at a speed of U. The lower wall was brought to a stop instantaneously at the beginning of the calculations. The channel height h is nondimensionalized by λ, the mean free path of the initial gas. Periodic boundary conditions are applied in the x- and z-directions. An artificial gravitational forcing (AF) is applied along the y-direction to the molecules.
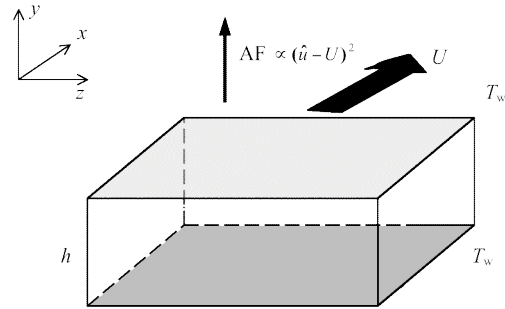

FIGURE 1. Forced model flow geometry.

$$\text{AF} = c\,(\hat{u} - U)^2 \qquad\qquad (1)$$

$\hat{u}$ represents the fluid velocity component in the x-direction. c denotes a constant coefficient that is used to adjust the level of the external forcing on the flow. A similar flow geometry and imposition of the artificial acceleration have been previously developed by Malek Mansour[11] in an analytical study of the onset of hydrodynamic instabilities and independently by Bird[12] to study the forced micro Couette flows. The effect of the artificial gravitational force is that, when a fluid particle is perturbed and moves in the y-direction, an effective buoyancy force favor further displacement of the particle in the y-direction. The scenario is similar to the instability mechanism associated with the centrifugal force in the Taylor-Couette and Görtler problems, where the Taylor-Görtler vortices have been observed in experiments and computed using two-dimensional DSMC. By using an artificial forcing in the form of Equation (1) instead of a physical one, it is possible to apply a wide range of forcing level to the flow without changing the flow geometry. Since the normalized root mean square of the disturbances is inversely proportional to the square root of the sample size,[13] the present flow model allows for a more efficient use of the computer resources in capturing unsteady, three-dimensional disturbances by artificially energizing the flow. It is reasonable to expect that vortical structures or flow patterns that are similar to the Taylor-Görtler vortices will also be found in the current model flow. In fact, earlier simulations[14,15] of the same flow geometry did capture highly organized discernable vortical mean flow structures. Fourier analyses of the vertical velocity signals show the existence of a hierarchy of fluctuation modes that consist of a fundamental and its harmonics. Up to six harmonics can be readily identified. In the following, results with different forcing coefficient will be presented and

compared for two different channel heights. The dynamics and the flow structural pattern of the sample averaged flow disturbances generated by the applied forcing will be examined.

RESULTS AND DISCUSSION

In this section, results of the simulations will be presented. The box height is 320. The parallel DSMC code used in this study has been validated by comparing with the serial code results of microchannel flows[2] and the results were reported.[3] For the present flow geometry, a comparison has also been made with the serial code results of Bird for a 2D domain that slices through the current box flow along a z-plane.[14] Flow patterns captured by the two codes were basically the same.

Two types of sampling have been used in the study to obtain macroscopic, averaged and disturbance components of the simulated flows. The "unsteady" properties, say for the vertical velocity component $\hat{v}$ is obtained by

$$\hat{v}(x,y,z,t) = \frac{1}{t_s}\int_{t-\frac{1}{2}t_s}^{t+\frac{1}{2}t_s}\sum_{i=1}^{M_c}c_{v,i}(t')\mathbf{d}t' \tag{2}$$

where c_v denotes the vertical component of the particle velocity, M_c the number of particle in the cell at time t'. t_s represents the short time period for the unsteady sampling. It was set at twenty times the mean collision time of the initial gas. The long-time-averaged or averaged component of the flow is obtained by

$$v = \frac{1}{t-t_0}\int_{t_0}^{t}\sum_{i=1}^{M_c}c_{v,i}(t')\mathbf{d}t' \tag{3}$$

where t_0 denotes the beginning time of the sampling. The difference between the unsteady sample average and the long time average is defined as the perturbation v'. Or,

$$v' = \hat{v} - v \tag{4}$$

The artificial forcing is applied in the three-dimensional simulations with a computational box of size 800×320×640. The box dimensions are nondimensionalized by the initial mean free path λ. The Knudsen number, based on the channel height h is 1/320. In the present three-dimensional simulation, 48 million particles were used. Typically, twenty processors were used. Depending upon the level of forcing and the box sizes, the computing time to achieve, for instance, stationary results are regularly in the order of two to three weeks. For the present simulations, the time steps are 20% of the mean molecular collision time of the initial gas (T_c). That is, $\Delta t^* = 0.2$. In a previous work,[15] it has shown that unsteady DSMC simulations are independent of their exact values as long as the time steps are small compared with the mean molecular collision time. It is valid for not only the stationary state of a flow but also its development in time. The speed U of the top plate is set equal to twice the most probable molecular speed c_{mp} at the initial gas temperature of 1,000 K. That is U=2. The Reynolds number is 1,156. The forcing level is changed by varying the value of c (=0.001, 0.01). The maximum forcing that can occur in the flow then varies by a factor of about 10. The results for the same flow geometry with different channel heights, plate speeds, and forcing constants have been shown in earlier work.[15,16] For comparisons with the results of the current simulations, some results with h=60, U=1, and c=0.04 from the previous simulations are shown in Figures 2 and 3. The computational box size is 800×60×320 and 16 million particles were used. The Knudsen number is 1/60. Figure 2 shows the long-time-averaged in-plane pathlines at three axial locations. The long time average begins at the initiation of the simulations. The mean flow pattern has reached a stationary state. The flow is periodic in the spanwise direction with three counter rotating vortical structures. The wavelength is 320/3. As is mentioned earlier, the vortical structures appear as a result of the externally applied forcing in the y-direction that mimics the centrifugal forcing in the Taylor-Couette problems. Figure 3a shows the energy spectra of the instantaneous (unsteady), the long-time-averaged, and the disturbance flow fields. The velocity component signals are taken at the cell that is located at the center of the simulation domain. Note that a disturbance has been defined in the present study in Equation (4) as the
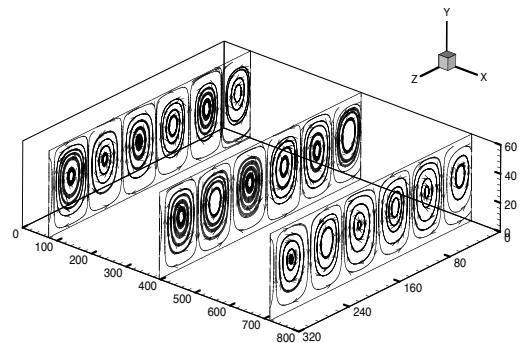

FIGURE 2. In-plane pathlines of the long-time-averaged flow for h=60, U=1, and c=0.04.

difference between the unsteady sample average and the long time average. Figure 3b shows the spectra of the cross correlation of the vertical and the spanwise velocity components. The long-time-averaged component of the instantaneous velocity field, which shows highly spatially coherent patterns (Figure 2), is temporally dominated by the zero frequency (=(m-1)/(20Tc)), or stationary mode. The spectrum distributions at other frequencies are flat, indicating that the signals are mainly statistical fluctuation at those frequencies. The correlation spectra show that the mean flow is highly correlated at zero frequency. The distributions of the disturbance correlation spectra are flat, indicating that there does not appear to be very strong correlations between the vertical and the spanwise disturbance velocity components.
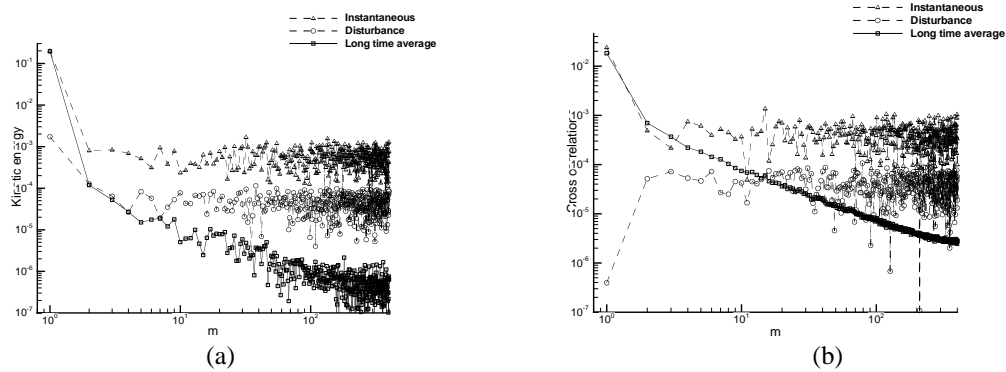
(a) (b)

FIGURE 3. Fourier spectra for h=60, U=1, and c=0.04. (a) Energy; (b) Cross correlation.

With the same flow conditions and parameters in the artificial forcing, more work is done to the particles in the larger flow domain of h=320 than those of h=60 and the flows are more energetic. For the h=320 cases that are shown in the following, the speed of the top plate U is set equal to 2 and c=0.001 and 0.01, respectively. Figure 4a shows the in-plane pathlines of the mean flow at three x-locations at tU/h=83.08, where the time scale h/U is about 320 Tc. The mean flow pattern has reached a stationary state. The periodic flow pattern has one pair of vortical structures in the mean flow in the spanwise direction. The time development of the flow shows that secondary flows,
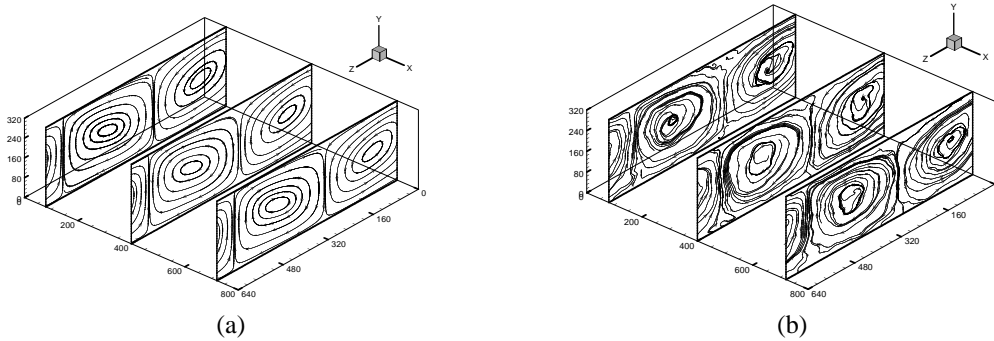
(a) (b)

FIGURE 4. In-plane pathlines. c=0.001. (a) Long-Time-Averaged flow; (b) Disturbances.

which did not exist in the initial conditions, first develop from the lower region of the flow, where the applied forcing is large. Flow structures with a large range of length scales then develop. At a later time, the small-scale flow patterns disappear. In a time sequence animation of the computed flow, the flow structures were seen evolving through events that involved the amalgamation, generation, and destruction of vortical structures, large and small. Figure 4b shows the in-plane pathlines for the disturbance flow on the same three planes in the x-direction as those in Figure 4a. Despite the statistical fluctuations, there are identifiable flow patterns that are vortical and similar in appearance with those shown in Figure 4a for the mean flow. Figure 5 shows the time history of the disturbance velocity
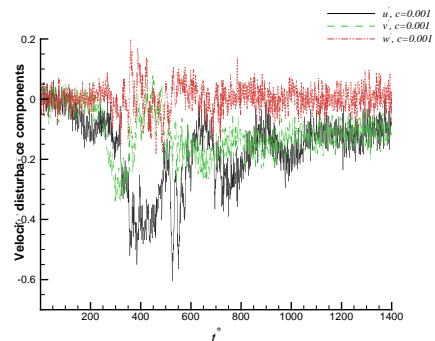
FIGURE 5. Evolutions of disturbance velocity components for c=0.001.

component signals at the cell that is located at the center of the simulation domain from the beginning of the simulation. The DSMC disturbance velocity signals contain statistical fluctuations about averages that appear to be stabilizing toward the end of the simulation. Figure 6a shows the energy spectra of the instantaneous (unsteady), the long-time-averaged, and the disturbance signals (shown in Figure 5). Figure 6b shows the spectra of the cross correlation of the vertical and the spanwise velocity components. The long-time-averaged component of the instantaneous velocity field, which shows highly spatially coherent patterns (Figure 4a), is temporally dominated by the stationary mode. The disturbance spectra contain regions of low to medium frequency with Fourier amplitudes that are at least two orders of magnitude higher than the statistical scatter apparent at the high frequency end of the spectra. The long-time-averaged and the disturbance kinetic energy spectra increase nearly linearly (in the log scale) toward the low frequency end. The correlation spectra at the low frequency are somewhat higher than the other modes that appear quite random.
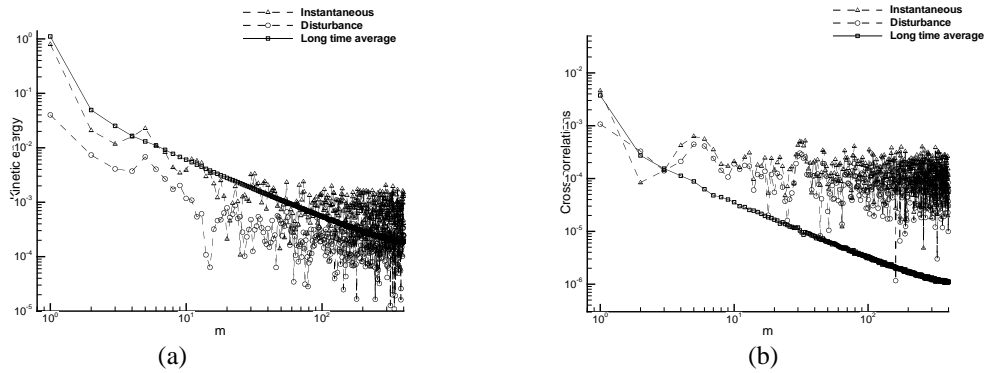

FIGURE 6. Fourier spectra for *c*=0.001. (a) Energy; (b) Cross correlation.

Simulations with *c*=0.01, which is ten times of that for the previous case, have also been performed. The larger forcing further energizes the flow. Figure 7a shows the in-plane pathlines of the flow disturbances. The disturbance flow pathlines are rather smooth, indicating that the resolved disturbances are not dominated by statistical fluctuations. The flow disturbances are vortical and are highly three-dimensional. The sizes of the three-dimensional vortical structures vary from as large as the channel height to very small. As the simulation proceeds, these structures go through mixed series of growth, amalgamation, and decay processes. Note that the secondary flow in the mean (not shown) and the three-dimensional disturbances do not exist in the initial conditions and the flow is not preferentially perturbed by any means in the DSMC simulations. Figure 7b shows the velocity
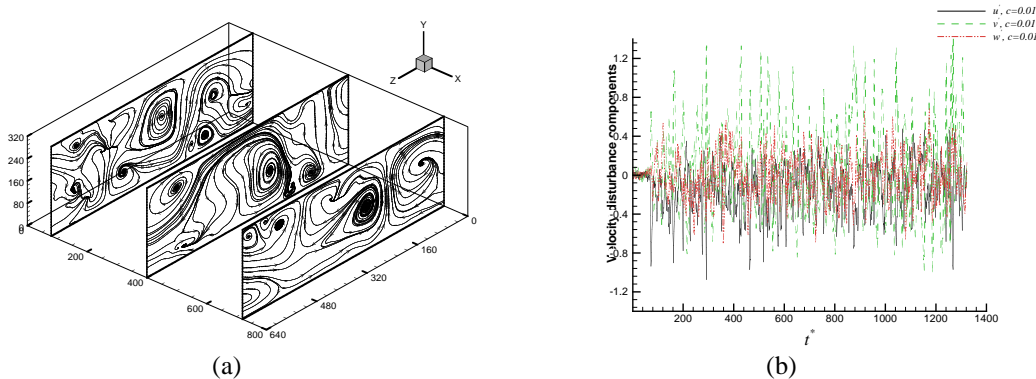

FIGURE 7. Flow disturbances for *c*=0.01. (a) In-Plane pathlines; (b) Velocity component signals.

disturbance signals registered at the center cell of the simulation domain. Compared to the disturbance signals shown in Figure 5 for *c*=0.001, the disturbance velocity components are larger in magnitude. The frequent occurrence of these large and small amplitude excursion reflects the evolution process of the disturbance flow structures given in Figure 7a. Figure 8 shows the kinetic energy and the correlation spectra from the velocity signal recorded at the center cell of the computational domain. For the mean flow, the spectrum for the zero-frequency mode is significantly higher than all the other modes. The disturbance kinetic energy spectra are high at the low and mid frequency range and drop off by more than one order of magnitude at the high frequency end. Similar drop-off in the spectra from the mid to high frequency modes by about one order of magnitude is also apparent in the velocity

correlation spectra shown in Figure 8b. These spectra show that the energetic modes of disturbances in the low to mid frequency correlate well and form the three-dimensional vortical structures shown in Figure 7a.
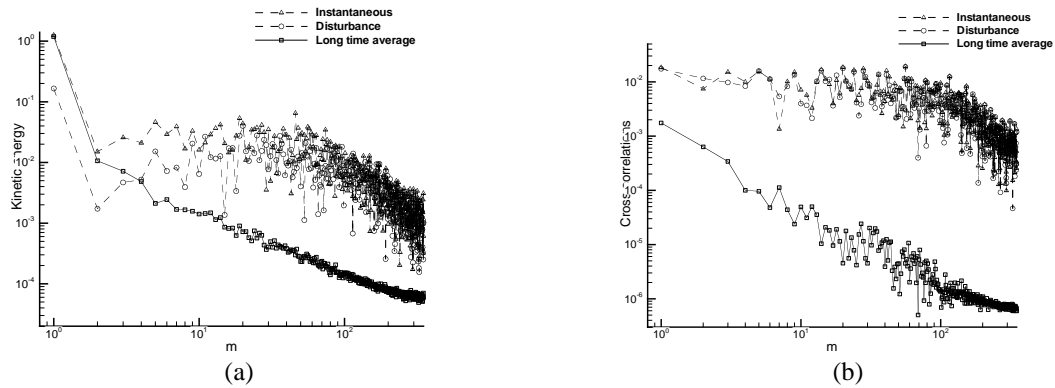

FIGURE 8. Spectra for c=0.01. (a) Energy; (b) Cross correlation.

CONCLUDING REMARKS

In addition to the mean flow, the unsteady DSMC simulations of the micro Couette flow, with sufficient artificial forcing, show clearly unsteady, three-dimensional flow disturbances that are coherent and well correlated both spatially and temporally. Since an artificial body force is applied to energize the system, the captured events may not be realistic. Nevertheless, it is evident from the present results that the DSMC method is capable of resolving oscillatory three-dimensional disturbances of physical significance. In a recent work, we examine the micro Rayleigh-Bénard problem where a physical buoyancy force naturally arises due to the temperature gradient and no artificial forcing is used. The preliminary results of the unsteady, three-dimensional DSMC simulations[17] show Rayleigh-Bénard cells in the mean flow and disturbances that are unsteady and three-dimensional. These findings suggest that unsteady DSMC can be used for the direct numerical simulations of the gas flows in microfluidic devices.

ACKNOWLEDGMENTS

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