JOURNAL OF THERMOPHYSICS AND HEAT TRANSFER
Vol. 12, No. 3, July–September 1998

Technical Notes

TECHNICAL NOTES are short manuscripts describing new developments or important results of a preliminary nature. These Notes cannot exceed 6 manuscript pages and 3 figures; a page of text may be substituted for a figure and vice versa. After informal review by the editors, they may be published within a few months of the date of receipt. Style requirements are the same as for regular contributions (see inside back cover).

Role of Boundary Conditions in Monte Carlo Simulation of Microelectromechanical Systems

Robert P. Nance*
North Carolina State University, Raleigh, North Carolina 27695-7910
David B. Hash†
NASA Ames Research Center, Moffett Field, California 94035
and
H. A. Hassan‡
North Carolina State University, Raleigh, North Carolina 27695-7910

Introduction

RECENTLY microelectromechanical systems (MEMS) have become the focus of a great deal of attention in several research disciplines. These devices are manufactured using processes similar to those used in microprocessor fabrication and promise the opportunity to sense and control physical processes at length scales on the order of a micron.[1] Potential applications for such devices cover a broad spectrum, including adaptive optics, surgical instruments, and laminar flow control. Many of these proposed designs involve fluid flow through microchannels, such as the use of microchannels to dissipate heat in integrated circuits.

Because of the very small length scales associated with MEMS devices, the fluid mean free path can be on the order of the characteristic channel dimensions. This fact indicates that treating the microchannel flow as a continuum phenomenon may lead to inaccurate results. Thus, these flows appear to be well-suited to the application of Bird's direct simulation Monte Carlo (DSMC) method.[2] However, microchannel simulations present a set of challenges not encountered in previous DSMC applications. First of all, the flow velocities in these systems are generally much less than the speed of sound. Consequently, the stream and vacuum boundary conditions typically employed in DSMC calculations are not physically appropriate. Instead, one must use inflow and outflow conditions that impose the correct propagation of information across the boundaries. This fact is now quite well established, and alternative DSMC boundary conditions for low-speed flows have been described in a number of sources.[3,4]

Secondly, microchannels are characterized by very large aspect ratios (ratio of channel length to channel height). One of the fundamental assumptions in the DSMC method is that the cell size in the gradient direction must be less than a fluid mean free path if the solution is to be considered valid. Proper resolution of both streamwise and transverse flow directions will lead to a large number of cells, implying that a single time step will be quite expensive to compute.

The preceding problem is aggravated by the need to compute a very large number of time steps before steady flow is attained. Generally, the length of the transient portion of a simulation is estimated by considering the amount of time necessary for a particle traveling at the mean flow velocity to traverse the computational domain. Because the domain size, i.e., channel length, is relatively large and the flow velocity is relatively small, the flow residence time will be considerably larger than in re-entry simulations. Moreover, operating conditions for such channels are typically near standard temperature and pressure, leading to a high collision frequency. A high collision frequency corresponds to a low mean collision time. Because DSMC also requires that the simulation time step be less than the mean collision time, the total number of time steps associated with the transient phase will be very large.

Finally, microchannel simulations require much larger run times than traditional problems, even after steady flow has been established. It has been pointed out that many microchannel flows involve mean flow velocities on the order of 0.1 m/s.[3] Thus, at ambient temperatures around 300 K, the ratio of the mean flow velocity to the average thermal speed can be on the order of 0.01% or even less. This extremely low signal-to-noise ratio has serious implications for DSMC because the method is probabilistic in nature. It is estimated that Monte Carlo simulation of realistic microchannels will require over 100 million steady-state samples to eliminate scatter from the results.

The main objective of this Note is to discuss the role of boundary conditions in MEMS simulations. Many of the other issues mentioned earlier were examined in Ref. 5. This investigation utilizes a parallel version of Bird's DSMC3 demonstration code.[2] Although the original algorithm was developed for three-dimensional simulations, only two-dimensional cases are considered here. A uniform Cartesian grid is used to minimize the time associated with particle movement, and parallelization is achieved through use of the CHAOS runtime library developed at the University of Maryland.[6] This library provides the programmer with simple procedure calls for data migration, domain decomposition, and dynamic load balance. CHAOS has already been shown to yield excellent parallel performance when coupled with the DSMC3 algorithm.[7]

To perform accurate microchannel solutions, new inflow and outflow boundary conditions were developed and incorporated into the basic algorithm. At the inflow boundary, we elect to specify the pressure, temperature, and transverse velocity (assumed to be zero for the present application). The streamwise velocity is determined for each boundary cell through consideration of the fluxes across the cell's boundary face and enforcing conservation of particles.

Presented as Paper 97-0375 at the AIAA 35th Aerospace Sciences Meeting, Reno, NV, Jan. 6–9, 1997; received Jan. 21, 1997; revision received Feb. 5, 1998; accepted for publication March 3, 1998.

*Research Assistant, Mechanical and Aerospace Engineering. Student Member AIAA.

†Research Scientist/Engineer, Thermosciences Institute. Member AIAA.

‡Professor, Mechanical and Aerospace Engineering. Associate Fellow AIAA.

For a given mean speed and temperature, the particle flux $\dot{n}$ across a boundary in a particular direction can be determined as follows, assuming a Maxwellian distribution[2]:

$$\dot{n} = \frac{nC_{mp}[\exp(-q^2) + \sqrt{\pi}q(1 + \text{erf}\, q)]}{2\sqrt{\pi}}, \qquad q = s\cos\theta \quad (1)$$

where s is the speed ratio V/C_{mp}, V is the mean speed, C_{mp} is the most probable speed, and θ is the angle between the velocity vector and normal to the boundary element. Considering the boundary face of inflow cell m, we can apply Eq. (1) to determine the flux crossing the face in either direction. Then, if particles are conserved

$$(\dot{n}_+ - \dot{n}_-)_m = n_i(u_i)_m A \quad (2)$$

where the subscripts + and − refer to particle fluxes in the positive and negative x directions, respectively, n is the number density and A is the area of the boundary face. Note that the inflow velocity depends on the incoming number flux, which in turn depends on the inflow velocity. Hence, Eq. (2) is actually a nonlinear function of the inflow velocity $(u_i)_m$. Instead of solving for $(u_i)_m$ numerically, though, we use the last computed value to evaluate the positive number flux. As a result, we can easily rearrange Eq. (2) to determine the new inflow velocity:

$$(u_i)_m = \frac{(\dot{n}_+ - \dot{n}_-)_m}{n_i A} \quad (3)$$

The value of $(u_i)_m$ will vary during the simulation. However, the velocity should eventually attain a nearly constant value in each inflow cell. The known inflow properties are then used to determine the entering particle distributions.

This inflow condition is quite similar to the subsonic boundary conditions proposed by Ikegawa and Kobayashi.[4] One important difference is that Ikegawa and Kobayashi use the particle-conservation concept to come up with a constant inflow velocity, whereas in this work particle conservation is applied on a per-cell basis. Additionally, the particle fluxes in this implementation are computed from the Maxwellian distribution. In contrast, Ikegawa and Kobayashi determine the particle fluxes by actually counting the number of particles crossing the computational boundary.

For the outflow, we appeal to the theory of characteristics, which is frequently used in continuum calculations to derive boundary conditions for subsonic flows. The use of the theory implicitly assumes the flow to be locally inviscid, adiabatic, and close to a perfect gas. Note that we can apply the theory of characteristics even though the flow is rarefied, because the conservation equations themselves still hold. In this case, we have employed Whitfield's characteristic formulation,[8] because it allows the specification of a constant exit pressure p. The resultant equations (for a Cartesian grid) are

$$(\rho_e)_m = \rho_m + \frac{p_e - p_m}{a_m^2} \quad (4)$$

$$(u_e)_m = u_m + \frac{p_m - p_e}{\rho_m a_m} \quad (5)$$

$$(v_e)_m = v_m \quad (6)$$

In the preceding relations, the subscript e signifies exit quantities; ρ is the density, v is the transverse velocity, and a is the local acoustic speed. Because the exit pressure is known, the new value of the exit temperature can then be determined using the perfect-gas law:

$$(T_e)_m = p_e/[(\rho_e)_m R] \quad (7)$$

As with the inflow conditions, the outflow properties are expected to vary during the simulation before settling out to steady values.

Results and Discussion

The algorithm described above was applied to the microchannel geometry and flow conditions shown in Fig. 1. The given dimensions correspond to a channel aspect ratio of 60, and O_2 was specified as the working gas. Additionally, the Knudsen number based on channel height ranges from about 0.02 at the channel inlet to about 0.05 at the channel exit. This range of Knudsen numbers suggests that the channel operates in the slip-flow regime.

One of the requirements for a successful DSMC application is that the cell size in the gradient direction be less than a mean free path, as stated earlier. However, this requirement does not give us any insight into how well-resolved the grid must be normal to the primary gradient direction. In channel flow, there are gradients in both the streamwise and transverse directions, but the gradients in the latter tend to be much greater. If high resolution is required in both directions for an accurate solution, simulation of very high-aspect-ratio microchannels will be virtually impossible. Thus, one important consideration is the degree of underresolution that can be tolerated in the streamwise direction.

To make such a determination, the test channel was first simulated using a fully resolved grid (cell size in each direction less than a mean free path). This solution required 2400 cells in the streamwise direction and 40 cells normal to the channel wall, and yielded a total of approximately 2.1 million simulated particles at steady state. Once this solution was complete, the grid in the x direction was coarsened by successively doubling the cell length. This procedure was repeated several times, and the results were compared to those for the baseline, fully resolved solution.

Figure 2 shows some representative results from this procedure. Pressure variation along the channel centerline is compared for three different levels of refinement in the streamwise direction. Note that there is a factor-of-32 difference between the resolution on the finest grid and on the coarsest. It is seen from Fig. 2 that the pressure distribution agrees very well on all three grids.

To illustrate the significance of correct boundary conditions on the solution, the coarsest-grid case was rerun using standard DSMC stream conditions for the inflow and outflow planes. To apply these conditions it is necessary to specify an inflow velocity. Based on the results shown earlier, a value of 20 m/s was selected. Figure 3 compares computed pressure distributions along the duct centerline for the subsonic boundary conditions and the conventional boundary conditions. It is obvious from this graph that use of the physically incorrect conditions results in an erroneous solution.

Figure 3 also shows results for this case computed using the subsonic boundary conditions proposed by Piekos and Breuer.[3]

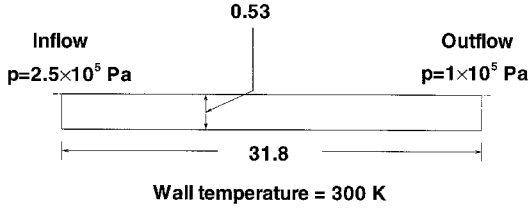

Fig. 1 Microchannel geometry considered in this work (dimensions in μm, not to scale).

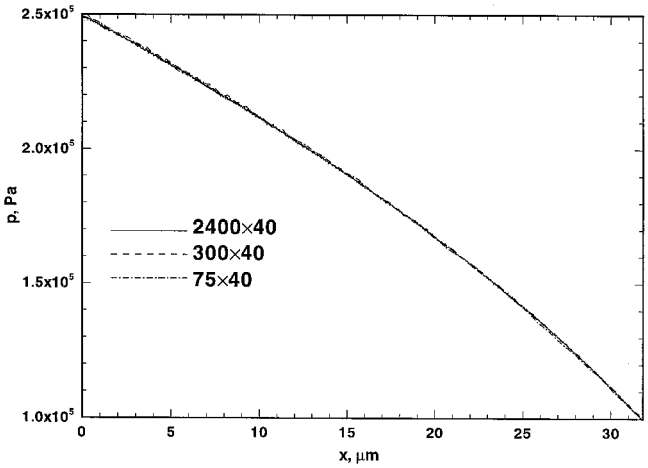

Fig. 2 Influence of grid resolution on centerline pressure distribution.

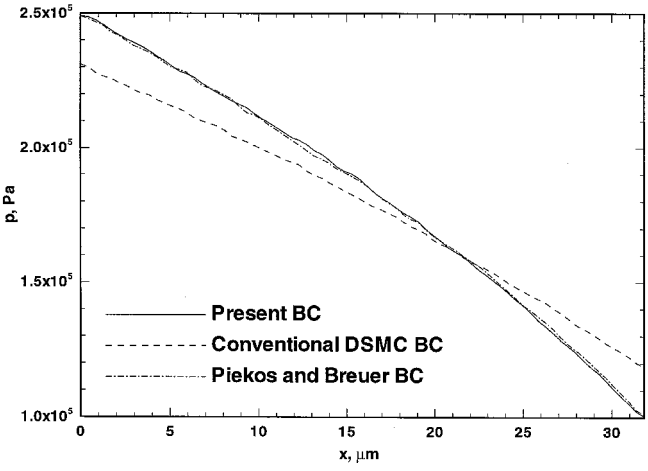

Fig. 3 Comparison of pressure distribution for new boundary conditions and standard DSMC boundary conditions.

This plot shows that results are virtually identical to those obtained with the boundary conditions proposed here. The agreement for other flow properties was found to be equally good.

In conclusion, we have proposed new DSMC boundary conditions suitable for use in low-speed MEMS applications. These conditions respect the proper directions of signal propagation for subsonic flows, and allow specification of inlet and exit pressures. Low-speed microchannel computations using these new conditions yield much better results than when traditional DSMC boundary conditions are used. However, the solutions are essentially the same as those obtained with the boundary conditions proposed by Piekos and Breuer.

Acknowledgments

This work was supported in part by NASA Cooperative Agreement NCC1-112 and a National Defense Science and Engineering Graduate Fellowship. Computer resources were provided by the Numerical Aerodynamic Simulation facilities at NASA Ames Research Center.

References

[1]Ho, C.-M., and Tai, Y.-C., "MEMS: Science and Technology," *Application of Microfabrication to Fluid Mechanics*, American Society of Mechanical Engineers, New York, 1994, pp. 39–49.

[2]Bird, G. A., *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Clarendon, Oxford, England, UK, 1994.

[3]Piekos, E. S., and Breuer, K. S., "DSMC Modeling of Micromechanical Devices," AIAA Paper 95-2089, June 1995.

[4]Ikegawa, M., and Kobayashi, J., "Development of a Rarefied Flow Simulator Using the Direct-Simulation Monte Carlo Method," *JSME International Journal*, Series 2, Vol. 33, No. 3, 1990, pp. 463–467.

[5]Nance, R. P., Hash, D. B., and Hassan, H. A., "Role of Boundary Conditions in Monte Carlo Simulation of MEMS Devices," AIAA Paper 97-0375, Jan. 1997.

[6]Hwang, Y. S., Moon, B., Sharma, S., Ponnusamy, R., Das, R., and Saltz, J., "Runtime and Language Support for Compiling Adaptive Irregular Problems on Distributed Memory Machines," *Software Practice and Experience*, Vol. 25, No. 6, 1995, pp. 597–621.

[7]Nance, R. P., Wilmoth, R. G., Moon, B., Hassan, H. A., and Saltz, J., "Parallel Monte Carlo Simulation of Three-Dimensional Flow over a Flat Plate," *Journal of Thermophysics and Heat Transfer*, Vol. 9, No. 3, 1995, pp. 471–477.

[8]Whitfield, D. L., "Three-Dimensional Unsteady Euler Equation Solutions Using Flux Vector Splitting," Dec. 1983.

Re-Examination of Double Diffusive Natural Convection from Horizontal Surfaces in Porous Media

C. T. Li* and F. C. Lai†
University of Oklahoma,
Norman, Oklahoma 73019-0601

Introduction

COUPLED heat and mass transfer as a result of buoyancy in saturated porous media is frequently encountered in engineering applications. From a fundamental perspective, Nield[1] made the first attempt to study the stability of convective flow in horizontal layers with imposed vertical temperature and concentration gradients. This was followed by Khan and Zebib[2] in the study of flow stability in a vertical porous layer. Bejan and coworkers[3,4] conducted a series of investigations of these effects on natural convection in enclosures filled with porous medium. Other geometries considered in the previous studies include line sources,[5] vertical surfaces,[6] horizontal surfaces,[7,8] vertical cylinders,[9] and slender bodies of revolution.[10] Among these previous studies, it is noticed that similarity solutions for coupled heat and mass transfer by natural convection from horizontal surfaces have been reported for a special case of constant wall temperature and concentration.[7,8] It is speculated that these solutions might not be physically plausible because they did not satisfy the conditions imposed on the velocity, boundary-layer thickness, local heat flux, and total heat convected as suggested by Gebhart et al.[11] Thus, the purpose of the present study is to reinvestigate this fundamental problem to determine the limits within which a physically realistic similarity solution exists. Emphases have also been placed on a fundamental examination of these double-diffusion effects on the flow, temperature, and concentration fields. It is expected that the obtained results will not only complement the current literature but also provide useful information for engineering applications.

Presented as Paper 97-2516 at the AIAA 32nd Thermophysics Conference, Atlanta, GA, June 23–25, 1997; received Aug. 25, 1997; revision received Feb. 16, 1998; accepted for publication Feb. 16, 1998.

*Graduate Research Assistant, School of Aerospace and Mechanical Engineering.

†Associate Professor, School of Aerospace and Mechanical Engineering. Senior Member AIAA.