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IP-DSMC method for micro-scale flow with temperature variation

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ABSTRACT

Based on the IP-DSMC method, a simple and effective temperature model is presented. By the developed IP-DSMC method with new temperature model, non-isothermal micro-flow is simulated. Comparing the developed IP results with the DSMC results, the correctness and effectiveness of the new temperature model are validated. Through simulating the orifice flow, it is found that it will cause numerical divergence if the second order central difference scheme of the mass conservation equation is used to update the information density when the local density gradient of the simulated flow is large. So the first order upwind scheme is recommended to update the information density.

1. Introduction

Microchannels are very important in many microelectrical mechanical systems (MEMS). Successful numerical simulation of the flow in these microchannels is required [1–3]. Here, microchannel flows are sometimes in the transition regime and rarefied effects are significant, so traditional continuum computational fluid dynamic (CFD) techniques are often invalid because CFD is based on the continuum assumption. The direct simulation Monte Carlo method (DSMC), proposed by Bird [4,5], can successfully simulate flows for molecular free flow and transition flow regimes because it is based on kinetic theory and does not rely on the continuum assumption. Some researchers [6–8] have already applied it to simulate microchannel flows. However, they have found it very difficult to obtain statistically convergent results under experimental conditions because of the statistical scatter, which makes DSMC simulation of microchannel flows extremely time-consuming. An information preservation (IP) [9,10] method has been proposed by Fan and Shen to address this issue. The IP method by Fan and Shen is highly effective in simulating the isothermal flow, but the IP method which can effectively simulate the non-isothermal flow is in the development and needs further deep research [10,11].

Based on the IP method, a simple and effective temperature model for micro-scale calculation is presented in this paper. The IP method with this new temperature model can simulate the non-isothermal flow effectively.

2. Computational method

2.1. Direct simulation Monte Carlo method

The DSMC method was introduced by Bird in the early 1960s to simulate rarefied gas flows. It is a numerical method to solve the dynamic equations for real gases using thousands or millions of simulated particles. Each simulated molecule represents a large number of real molecules. The DSMC method only considers the binary collisions, so the molecular motion

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and their collisions are uncoupled when the computational time step is smaller than the physical collision time. At the beginning of the calculation, the simulated molecules are uniformly distributed statistically in the cells. At each step, all molecules move according to their individual velocities. As the simulated molecules move, they may collide with the other simulated molecules or interact with the physical boundaries. In this process, both momentum and energy are conserved. In each cell, collision pairs are selected and collisions are calculated. These steps are repeated until the statistical scatters are small enough. Finally, the macroscopic characteristics of the flow are obtained by sampling the molecular properties in each cell.

2.2. Information preservation method

The IP method, first proposed by Fan and Shen, is used to overcome the problem of statistical scatter in low-speed flow systems. It assigns each simulated molecule in the DSMC method two velocities. One is the thermal velocity used to compute molecular motion following the same steps as the DSMC method. The other is called information velocity; which corresponds to the collective velocity of the enormous number of real molecules that the simulated molecule represents. Macroscopic velocity and shear stress are computed from the information velocity to remove the statistical scatter source inherent in the DSMC method due to the randomness of the thermal velocity. A preliminary study [9] described the IP method in details. With the constant temperature assumption, the initial IP method is not appropriate to simulate the non-isothermal flow, so researchers are improving the temperature model in order to simulate the non-isothermal flow.

2.3. The developed IP method

2.3.1. Information temperature

For the absolute value of the temperature in microchannel flows is large and the fluctuation of the temperature is small, in the developed IP method, Eq. (1) is used in the Step (5) in the study [9] to update information cell temperature.

$$T_l = \frac{1}{5}(T_{i-1,j} + T_{i+1,j} + T_{i,j} + T_{i,j-1} + T_{i,j+1}). \tag{1}$$

The grid which Eq. (1) corresponds to is shown in Fig. 1. $T_{i,j}$ is the cell temperature. Eq. (1) can effectively decrease the fluctuation of the cell temperature. This temperature model can successfully simulate the non-isothermal flow.

In the simulation, the information pressure p_i and cell pressure p_l are obtained by gas state equation. The decrease of the cell temperature fluctuation will be benefit for the decrease of the cell pressure fluctuation. The cell pressure p_l is used to calculate the force of the cell shown in Eq. (2).

$$F_l = \sum_{k=1}^{2\phi} p_l^k A_l^k n_l^k + f_l V_l, \tag{2}$$

where p_1^k is the k surface pressure of the cell l, A_l^k and n_l^k are the surface area and unit normal vector of the k surface, respectively. f_l is the body force of the cell l and V_l is the cell volume. The acceleration of simulated molecules can be expressed by the Eq. (3).

$$a_l = \frac{F_l}{\rho_l V_l}. \tag{3}$$

The velocity variation of the simulated molecules is $a_l \Delta t$. So the velocity of simulated molecules is changed by the variation of information cell temperature. And then the effect of fluid temperature on the information velocity can be indirectly reflected in the simulation.

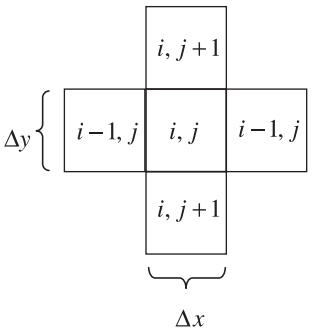

Fig. 1. The grid of the IP method.