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Subsonic flow boundary conditions for the direct simulation Monte Carlo method

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ABSTRACT

The performance of different types of boundary conditions used in direct simulation Monte Carlo models of subsonic flows for single species flow fields is assessed in this study. An inlet boundary condition that permits the specification of pressure and temperature is investigated, as well as one that permits the specification of mass flow rate and temperature. A new inlet boundary condition is suggested that permits the total mass flow rate to be specified without requiring inter-processor communication during a parallel computation. Two types of outlet boundary conditions are investigated, one in which the outlet pressure is maintained by controlling the porosity of the outlet surface, and another in which particles are introduced at the outlet with properties such that the desired pressure is maintained. Each of the boundary conditions investigated produce flow field results for a single species, microchannel flow that are in good agreement with an analytical solution of the flow field and previously reported results. However, a simulation of a more complicated multi-species flow inside a vapor deposition reactor shows that some of the predicted flow field and surface properties are a function of the type of outlet boundary condition used.

1. Introduction

Physical Vapor Deposition (PVD) and Chemical Vapor Deposition (CVD) processes are commonly used for semiconductor wafer processing, microfabrication processes and in other applications where thin films are needed. Many of these processes are operated at low pressures and involve flows over features with small length scales [1]. These operating characteristics can result in an insufficient number of collisions between gas particles to maintain an equilibrium velocity distribution everywhere in the device, placing the associated flow fields in the transitional or non-continuum flow regimes. The direct simulation Monte Carlo (DSMC) method [2] is appropriate for the simulation of these types of flows, which are in translational nonequilibrium.

Since the DSMC method was originally developed for the simulation of external, hypersonic flow fields, new physical models are required in order to simulate the type of environments that are encountered in materials processing applications. One of the most obvious requirements is the need for boundary conditions that are appropriate for the simulation of subsonic flows. When modeling a hypersonic flow field using DSMC, one is free to specify all macroscopic flow field properties at the hypersonic inlet, and none at the outlet, since the flow at both boundaries is supersonic. These are the so-called "stream" and "vacuum" boundary conditions that are used in DSMC simulations of external, hypersonic flow fields. In contrast, at the inlet boundary of a subsonic flow, information about one of the macroscopic flow properties must not be uniquely specified. Instead, it must come from the inside of the domain. At an outflow boundary of a subsonic flow, only one of the macroscopic flow properties can be specified; all other information about the boundary must be obtained from inside the flow domain. These requirements are a result of the direction of information travel in the flow field; a more in-depth discussion of these requirements is found in Ref. [3].

A number of DSMC studies have been reported for problems that involve subsonic flow, for example, in microchannels and microtubes, MEMS devices, and materials processing devices such as CVD reactors. These previous studies involved the use of a variety of techniques to prescribe subsonic flow at inlet and outlet boundaries, and the level of detail presented concerning the method of implementation of the boundary conditions varies in these reports. The authors are not aware of a study that is focused solely on the implementation details, and performance comparison of, subsonic boundary conditions for DSMC simulations. Thus, the goal of this study is to summarize and present the implementation

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details of four types of previously reported subsonic boundary conditions, validate them by simulating a single species flow inside a microchannel for which an analytical solution of the flow field exists, and assess their ability to model a more complicated, multi-species flow inside a deposition reactor. We focus in this work solely on obtaining steady-state solutions to the systems considered, and therefore do not consider time-dependent boundary conditions.

The outline of the paper is as follows. First, a brief overview of the DSMC method is given, followed by a review of the types of subsonic boundary conditions for the DSMC method that have been presented in the literature. A new subsonic inlet boundary condition is presented, which allows the specification of total mass flow rate at the inlet, but does not require communication between different processors during a parallel simulation. Next, various combinations of subsonic inlet and outlet boundary conditions are used to simulate the flow in a two-dimensional microchannel, and the results are compared to an analytical solution for the flow field. The generality of the boundary conditions is then demonstrated by applying them to the axisymmetric simulation of the flow field in a portion of a showerhead reactor that might be used for PVD or CVD processing of materials. Lastly, conclusions about the performance and limitations of the different types of boundary conditions are drawn.

2. Numerical method

The DSMC method is the most versatile computational technique currently available to simulate rarefied gas flows, because physical models for interaction of multiple species, gas-phase chemical reactions, gas-surface interaction, and internal energy exchange are readily incorporated into the method. The basic ideas of the DSMC method are summarized as follows. Each simulator particle has a mass, velocity, and (if applicable) internal energy, and represents a large number of real gas particles. The movement of the particles through the computational mesh and the collisions between particles are performed independently, which places restrictions on the maximum value of computational time step and mesh cell size that can be used in the simulation. Collisions between particles are performed stochastically, and the dilute gas assumption is made so that only binary collisions are considered. The simulation begins from a specified initial condition, and iterations are performed in which particles collide, move, and enter and leave the domain through the boundaries, while the flow field evolves to a steady state. Once a steady state has been reached, macroscopic flow field properties such as temperature and velocity are obtained by performing the appropriate averages over the particles in each cell of the computational mesh. The DSMC method is described in detail in Ref. [2].

In the current study, an existing DSMC code is used that has been extensively verified and validated [4–6]. The No Time Counter technique [2] and the Variable Hard Sphere (VHS) model [2] are used to simulate collisions between particles. All wall surfaces are modeled as diffusely reflecting. A structured, quadrilateral mesh is used for the simulations of the two-dimensional microchannel flow, while an unstructured, triangular mesh is used for the simulations of the axisymmetric showerhead reactor flow.

In axisymmetric DSMC simulations, the dependence of cell volume on distance from the axis of symmetry leads to a large variation in cell volumes throughout the grid. This can result in cells far from the axis containing undesirably large numbers of simulator particles, increasing the computational cost of the simulation unnecessarily [7]. In this work, spatially varying weight factors are used to improve the numerical efficiency of the simulation of the showerhead reactor, by periodically modifying cell-based numerical weight values to achieve an average of one hundred simulator particles in each cell. To minimize the number of clone and destroy operations associated with this numerical weight variation, weight values in different cells are constrained to differ by some factor of two, and a smoothing operation is performed to limit the surface area of boundaries between different regions of uniform weight.

3. Boundary conditions for DSMC simulations

3.1. Inlet

The discussion of the inlet boundary conditions that follows assumes, without loss of generality, that the problem is defined such that the inlet surface is normal to the x-component of the mean velocity vector, that is, the velocity vector at the inlet is (U,0,0). However, the implementation of the boundary conditions described in this work is easily extended for use with arbitrarily oriented boundary surfaces by considering the component of the inflow vector that is normal to the boundary face.

Two types of inlet boundary conditions have been presented in the literature for single species flows; one in which the pressure and temperature of the incoming flow is specified, and one in which the total mass flow rate and temperature is specified. In this work, these types of boundary conditions are referred to as Type 1 and Type 2 inlet boundaries, respectively. In the implementation of both types of inlets, one piece of information about the macroscopic state of the gas at the inlet must be obtained from the interior of the computational domain.

Various implementations of the Type 1 boundary condition are described in the literature. In all cases, information about the streamwise velocity is taken from inside the computational domain. The method in which this is accomplished can be classified into three different categories: instantaneous calculation of the average velocity of simulator particles crossing the inlet boundary [8–10], use of the continuum characteristic line method to compute the streamwise velocity at the location of the inlet boundary [11], and zeroth order extrapolation of the velocity in each cell along the inlet to the location of the inlet boundary [12,13]. A derivation of pressure-based subsonic inlet boundary conditions based on the local one dimensional inviscid (LODI) formulation used in continuum flow computations was recently presented in Ref. [3] for use with the DSMC method. It was also shown in this work that the previously published boundary conditions that were based on the continuum characteristic line method can be derived from the LODI formulation. Each of these approaches involves describing the flow through the inlet boundary using a Maxwellian velocity distribution. Additionally, the continuum characteristic line method utilizes the assumption of continuum, inviscid flow to calculate the mean streamwise velocity at the inlet.

The specific implementation of the Type 1 boundary condition chosen for investigation in this work utilizes a zeroth order extrapolation of the streamwise velocity from each of the cells along the inlet to define the mean velocity of the particles that are injected at the inlet. The instantaneous, streamwise velocity in each cell along the inlet boundary is obtained by calculating the average of the streamwise velocity component of each individual particle in the cell,

$$u' = \frac{1}{N_p}\sum_{p=1}^{N_p} u_p, \tag{1}$$

where N_p is the number of particles in the cell under consideration and u_p is the streamwise velocity component of a particle. Because DSMC is a stochastic method, the instantaneous values of the macroscopic velocity in the cell fluctuate about the mean. The