Parallel Simulation of Microflows By DSMC and Burnett Equations

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PARALLEL SIMULATION OF MICROFLOWS BY DSMC AND BURNETT EQUATIONS

by

Yichuan Fang

A Dissertation
Submitted to the
Faculty of The Graduate College
in partial fulfillment of the
requirements for the
Degree of Doctor of Philosophy
Department of Mechanical and Aeronautical Engineering

Western Michigan University
Kalamazoo, Michigan
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The primary objective of this dissertation is to numerically simulate and study the heat transfer and flow characteristics in fluidic microelectromechanical system (MEMS). In typical microfluidic MEMS applications, the ratio of the gas mean-free-path to the characteristic length scale, or the Knudsen number, can be large. The traditional mathematical models of continuum fluid based on the Navier-Stokes equations may become invalid because of their constitutive relations of viscous stress and heat flux.

In this study, the direct simulation Monte Carlo (DSMC) method and the conventional Burnett equations are applied to model the microflows in microchannels from molecular and continuum point of view, respectively. The DSMC method has been implemented for a distributed parallel-computing environment with an excellent parallel efficiency. The Knudsen number effects on the viscous stress and heat transport are simulated and analyzed. The results of the microfluidic flow simulations show significantly different flow characteristics and heat transfer behavior compared with macroscale phenomena.

In addition, a parallel unsteady DSMC algorithm is also developed to study the time-dependent behavior of an initially chaotic micro-Couette flow. The results of the simulations show that the particle-based DSMC method has the capability to capture the nonlinear evolution of harmonic waves.
ACKNOWLEDGMENTS

The work of this dissertation was carried out with the help and encouragement of many people. First, I sincerely thank my advisor, Dr. William W. Liou, for his guidance, insight, advice and support throughout this research. It has been an honor and privilege working with him.

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Yichuan Fang
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CHAPTER I

INTRODUCTION

Motivations

The primary motivation of this research comes from the effort in simulating
the heat transfer characteristics and flowfield of the microfluidic flows in Micro-
Electro-Mechanical Systems (MEMS) using molecular- and continuum- based
computational fluid dynamics (CFD). The usual CFD codes, which have been
developed mainly for flows in the continuum regime, become inaccurate for the
microfluidic flows beyond continuum regime. The first principle particle simulation,
direct simulation Monte Carlo (DSMC), is one of the most accurate methods. But it is
computationally expensive, especially for high-density flows and large-scale
problems. It is also necessary to develop a continuum- based approach, solving
Burnett equations, for flows in the near-continuum regime. In order to improve the
computing capability, both of the algorithms for DSMC and Burnett equations are
parallelized.

The major physical issue in studying the microfluidic flows in MEMS is the
translational nonequilibrium effects on the viscous stress and heat flux within the
rarefied gas flow. In many MEMS applications, the mean-free path of the gas, \( \lambda \), is
comparable to the characteristic length scale, \( \ell \), of the devices. The rarefied gas
effects deviated from the equilibrium state of continuum are correlated with the Knudsen number, $Kn$, which is defined as

$$ Kn = \frac{\lambda}{\ell} $$  \hspace{1cm} (1.1)

The relations of the viscous stress and heat flux to gradients of flowfield variables (the constitutive relations) in many MEMS are different from those in large-scale devices (Liou and Fang 2001b). The constitutive relations for the flow of large-scale devices are those included in the Navier-Stokes equations, i.e. the linear Stokes law for the viscous stress and linear Fourier law for the heat flux. However, as the Knudsen number increases in MEMS, the fluid deviates more and more away from the equilibrium. As a result, the linear constitutive relations of the Navier-Stokes equations become less and less accurate, and nonlinear and higher order terms are needed in the constitutive relations. The Burnett equations have nonlinear and second order terms, expressed in terms of the Knudsen number, which were derived from the Boltzmann equation by using the kinetic theory of dilute gases (Chapman and Cowling 1970). The Boltzmann equation is the governing equation for the entire continuum-transition regime of MEMS. Therefore, the Burnett equations can better describe the flows in the near-continuum regime than Navier-Stokes equations.

The DSMC method was derived from the same first principles as the Boltzmann equation, but not from the equation itself. The Boltzmann equation can be derived through the DSMC procedures (Bird 1970). Unlike the Boltzmann equation, the DSMC algorithm does not depend on the existence of inverse collisions that are dictated by the symmetric binary collision dynamics. This allows the application of
DSMC to complex phenomena such as ternary chemical reactions that are inaccessible to the Boltzmann equations (Bird 1994). The DSMC method is accurate within the range where the Boltzmann equation works and can properly model the nonlinear and high-order terms of viscous stress and heat flux in microfluidic flows of MEMS.

Simulation of the microfluidic flows has become an emerging technology since the end of the last century. The rapid progress in fabricating and utilizing MEMS during the last decade has not been matched by corresponding advances in our understanding of the unconventional physics involved in the operation and manufacture of micro-devices. Providing such understanding is crucial to designing, optimizing, fabricating and operating improved MEMS devices.

**MEMS Development**

Micro-Electro-Mechanical Systems (MEMS) are a relatively new area of research, which have been developed rapidly in the last decades. MEMS refer to devices that have characteristic lengths from micrometers to millimeters, combining electrical and mechanical components. They are fabricated using integrated circuit (IC) batch-processing technology. These systems can sense, control, and actuate on the micro scale, and function individually or in arrays to generate effects on the macro-scale. The mechanical devices typically require more complicated process than the electrical devices.

As is summarized by Gad-el-Hak (2002), microfabrication techniques have been developed fast to create extremely small devices in recent years (Angell et al.
1983; Gabriel et al. 1988, 1992; O'Connor 1992; Bryzek et al. 1994; Ashley 1996; Ho and Tai 1996, 1998; Madou 1997; Knight 1999; Epstein 2000; Tang and Lee 2001). The books by Madou (1997) and Kovacs (1998) provide excellent sources for microfabrication technologies. Current manufacturing techniques for MEMS include surface silicon micromachining, bulk silicon micromachining, lithography, electrodeposition and plastic molding, and electrodischarge machining. Electrostatic, magnetic, electromagnetic, pneumatic and thermal actuators, motors, valves, gears, cantilevers, diaphragms and tweezers less than 100 μm in size have been fabricated. These have been used as sensors for pressure, temperature, mass flow, velocity, sound, and chemical composition; as actuators for linear and angular motions; and as simple components for complex systems such as robots, micro-heat-pumps and micro-heat-engines (Lipkin 1993; Garcia and Sniegowski 1993, 1995; Sniegowski and Garcia 1996; Epstein and Senturia 1997; Epstein et al. 1997).

MEMS are an enabling technology, finding increased applications in a variety of industrial and medical fields, with a potential worldwide market in the billions of dollars. Accelerometers for automobile airbags, keyless entry systems, dense arrays of micromirrors for high-definition optical displays, scanning electron microscope tips to image single atoms, micro-heat-exchangers for cooling of electronic circuits, reactors for separating biological cells, blood analyzers and pressure sensors for catheter tips are but a few of current usage. Microducts are used in infrared detectors, diode lasers, miniature gas chromatographs and high-frequency fluidic control systems. Micropumps are used for ink jet printing, environmental testing and electronic
cooling. Potential medical applications for small pumps include controlled delivery
and monitoring of minute amount of medication, manufacturing of nanoliters of
chemicals and development of artificial pancreas. Several new journals are dedicated
to the science and technology of MEMS. They include IEEE/ASME Journal of
Microelectromechanical systems, Journal of Micromechanics and Microengineering,
and Microscale Thermophysical Engineering.

What are the advantages of MEMS devices over current devices that perform
the same functions? There are many:

• MEMS devices can be so small that hundreds of them can fit in the same space as
one single macro-device that performs the same function.

• Cumbersome electrical components are not needed, since the electronics can be
placed directly on the MEMS device. This integration also has the advantage of
picking up less electrical noise, thus improving the precision and sensitivity of
sensors.

• Using IC processes, hundreds to thousands of these devices can be fabricated on
a single wafer. This mass production greatly reduces the price of individual
devices. Thus, MEMS devices will be much less expensive than their macro-
world counterparts.

For many applications, MEMS is sure to be the technology of the future, and is nearly
the technology of the present.
Flow Physics in MEMS

This work focuses on the MEMS that involve microfluid flows. Micronozzles, microchannels, micropumps, microturbines, and microvalves are examples of small devices involving the microfluid flows. Fluid flows in small devices differ from those in macroscopic machines. The operation of MEMS-based channels, nozzle, valves, bearings, turbomachines, etc., can not always be predicted from conventional flow models such as the Navier-Stokes equations with no-slip boundary conditions at the fluid-solid interface, as routinely and successfully applied to larger flow devices. Many questions have been raised when the results of experiments with microdevices could not be explained via traditional flow modeling. The pressure gradient in a long microchannel was observed to be non-constant and the measured flow rate was higher than that predicted from the conventional continuum flow model. Load capacities of microbearings were diminished and electric currents needed to move micromotors were extraordinarily high. The dynamic response of micromachined accelerometers operating at atmospheric conditions was observed to be over-damped.

In the early stages of development of this new field, the objective was to build MEMS devices as productively as possible. Microsensors were reading something, but not many researchers seemed to know exactly what. Microactuators were moving, but conventional modeling could not precisely predict their motion. After a decade of unprecedented progress in MEMS technology, perhaps the time is now ripe to take stock, slow down a bit and answer the many questions that arose. The ultimate aim of this long-term exercise is to achieve rational design capability for useful microdevices.
and to be able to characterize definitively and with as little empiricism as possible the operations of microsensors and microactuators.

For dilute gases, the mean free path $\lambda$ is the average distance traveled by molecules between collisions. For an equilibrium gas with a hard sphere model, the mean free path is $\lambda = \frac{1}{l(\sqrt{2} \pi d^2 n)}$ (Bird 1994). The mean free path can be transformed to an expression related to the temperature $T$ and pressure $p$ as follows

$$\lambda = \frac{kT}{\sqrt{2\pi d^2}}$$

(1.2)

where $d$ the molecular diameter, and $k$ the Boltzmann constant ($1.38 \times 10^{-23}$ J/K molecules). The Navier-Stokes equations are valid when $\lambda$ is much smaller than a characteristic flow dimension $\ell$; i.e., $Kn$ is small. As this condition is violated, the flow is no longer near equilibrium and the linear relation between the stress and the rate of strain and the no-slip velocity condition are no longer valid. Similarly, the linear relation between the heat flux and the temperature gradient and the no-jump temperature condition at a solid-fluid interface are no longer accurate when $Kn$ is not very small. The length-scale $\ell$ can be some overall dimension of the flow, but a more precise choice is the length scale of macroscopic properties, for example density $\rho$

$$\ell = \frac{\rho}{d \rho/d x}$$

(1.3)

The ratio between the mean free path and the characteristic length is known as the Knudsen number, which was shown in equation (1.1). Generally the traditional requirement for Navier-Stokes equations to be valid is that the Knudsen number should be less than 0.001 (Gad-el-Hak 1999).
The Reynolds number and Mach number are important characteristic parameters in macroscopic fluid mechanics. The Knudsen number can be expressed in terms of those two. The Reynolds number is the ratio of inertial force to viscous one

$$Re = \frac{u_0 \ell}{\nu}$$  \hspace{1cm} (1.4)

where $u_0$ is a characteristic velocity, and $\nu$ the kinematic viscosity of the fluid. The Mach number is the ratio of flow velocity to the speed of sound

$$Ma = \frac{u_0}{a_0}$$  \hspace{1cm} (1.5)

which is a measure of fluid compressibility and may be considered as the ratio of inertial force to elastic one. From the kinetic theory of gases, the mean free path is related to the viscosity as follows

$$\nu = \frac{1}{2} \lambda \bar{c}$$  \hspace{1cm} (1.6)

where $\bar{c}$ is the mean molecular speed with a relation with the sound speed $a_0$ as follows

$$\bar{c} = \sqrt{\frac{8}{\pi \gamma}} a_0$$  \hspace{1cm} (1.7)

where $\gamma$ is the specific heat ratio (i.e. the isentropic exponent). Combining Equations (1.6) and (1.7) to equation (1.1) yields,

$$Kn = \frac{\sqrt{\frac{\pi \gamma}{2}} Ma}{Re}$$  \hspace{1cm} (1.8)

In dealing with microfluid flows through microdevices, one is faced with the question of which model to use, which boundary condition to apply and how to
proceed to obtain solutions to the problem at hand. Obviously surface effects dominate in small devices. The surface-to-volume ratio for a machine with a characteristic length of 1m is 1m\(^{-1}\), while that for a MEMS device having a size of 1\(\mu\)m is 10\(^6\)m\(^{-1}\). The million-fold increase in surface area relative to the mass of the minute device substantially affects the transport of mass, momentum and energy through the surface. The small length-scale of microdevices may invalidate the continuum approximation altogether. Slip flow, thermal creep, rarefaction, viscous dissipation, compressibility, intermolecular forces and other unconventional effects may have to be taken into account, preferably using only first principles such as conservation of mass, Newton’s second law, and conservation of energy, etc.

Compressibility is another characteristic feature to recognize for some MEMS flows. The macroflows are usually treated as incompressible if the local Mach number is less than 0.3. But the well-known criteria, \(Ma < 0.3\), is not sufficient to allow treatment of a flow as incompressible. For instance, strong wall heating or cooling may cause the fluid density to change sufficiently and the incompressible approximation to break down, even at low speeds. As in flows in large-scale devices, the pressure changes due to inertia are indeed negligible at small Mach numbers. But the pressure changes in some microdevices can be mostly due to the strong viscous effects, as is the case of a long microchannel, where pressure changes may be significant even for flows with a low Mach number. Density then may change significantly and the flow must be treated as compressible. The heat transfer on the wall of microdevices may also affect the density changes. Not much is known about
the flow compressibility in MEMS.

In this work, molecular- as well as continuum- based fluid models and their applications to microfluid flows are discussed. The surface-boundary velocity slip, temperature jump, viscous effects as well as the compressibility effects have been studied through the direct simulation Monte Carlo. This molecular-based method makes use of the well-developed kinetic theory of gases, embodied in the Boltzmann equations. Burnett equations are also solved with modeled boundary conditions of velocity-slip/temperature-jump.

Microfluidic Modeling

A gas flow may be modeled at either the microscopic or the macroscopic level (i.e., molecular-based vs. continuum-based models). The former presents fluid by a collection of particles, and the latter by continuum. The molecular-based models are subdivided into deterministic and statistical methods. The molecular dynamics (MD) method is the best-known deterministic simulation approach, while the starting point in statistical mechanics is the Liouville equation. The Liouville equation expresses the conservation of the N-particle distribution function in 6N-dimensional phase space, which consists of velocity space and physical space. In the continuum-based models the velocity, density, pressure, and temperature, etc., are defined at every point in space and time, and conservation of mass, momentum and energy lead to a set of nonlinear partial differential equations (Euler, Navier-Stokes and Burnett equations, etc.). The classification for fluid modeling is depicted schematically in Figure 1.
Figure 1. Molecular and continuum fluid models. MD: molecular dynamics; EHE: extended hydrodynamic equations; THE: traditional hydrodynamic equations; LGCA: lattice-gas cellular automata.

The continuum model of Navier-Stokes equations is applicable to many common flow situations. It ignores the molecular nature of fluid and regard the fluid as a continuous medium describable in terms of the spatial and temporal variations of density, velocity, pressure and other macroscopic flow variables. For dilute gas flows near equilibrium, the Euler and Navier-Stokes equations are derivable from the molecular-based Boltzmann equation, but can also be derived independently for both liquids and other dense gases. The continuum model is easier to handle mathematically and computationally more efficient than the alternative molecular models. Continuum model should therefore be used as long as it is applicable.
Basically, the Navier-Stokes equations lead to fairly accurate solutions as long as the following two conditions are satisfied. One is that local properties such as density and velocities can be defined as averages over elements large compared to the microscopic structure of the fluid but small enough in comparison with the scale of the macroscopic phenomena to permit the use of differential calculus to describe them. The other is that the flow must not be too far from thermodynamic equilibrium. The former condition is almost always satisfied, but the latter usually restricts the validity of the Navier-Stokes equations. As will be seen in the next chapter, the continuum flow model does not form a determinate set. The shear stress and heat flux must be expressed in terms of lower-order macroscopic variables such as velocities and temperature, and the linear relations are valid only when the flow is near thermodynamic equilibrium. Also, the traditional conditions of velocity no-slip/temperature no-jump at a solid-fluid interface breaks down even before the linear stress-strain relation becomes invalid.

The flows in microdevices such as MEMS at normal atmosphere have rarefied-gas effects, just as the rarefied gas flows in the high-altitude flying vehicles with low pressure. The value of the local Knudsen number in a particular flow determines the degree of rarefaction and the degree of validity of the continuum models. In 1909 Knudsen performed the pioneering experiments in rarefied gas dynamics. The different Knudsen number regimes are determined empirically and are therefore only approximate for a particular flow. In the limit of zero Knudsen number, the transport terms in the continuum momentum and energy equations are negligible.
and the Navier-Stokes equations then reduce to the inviscid Euler equations. Both heat conduction and viscous diffusion and dissipation are negligible, and the flow is then approximately isentropic (i.e. adiabatic and reversible) from the continuum viewpoint while the equivalent molecular viewpoint is that the velocity distribution function is everywhere of the local equilibrium or Maxwellian form. As $Kn$ increases, rarefaction effects become more obvious, and eventually the continuum approach breaks down altogether. The different Knudsen number regimes and its limits on the micro-gas modeling are described in Figure 2, and can be summarized as the following (Gad-el-Hak 1999),

- **Euler:** $Kn \rightarrow 0$ ($Re \rightarrow \infty$)
- **Navier-Stokes without slip boundary:** $Kn < 10^{-3}$
- **Navier-Stokes with slip boundary:** $10^{-3} \leq Kn < 10^{-1}$
- **Continuum-transition regime:** $10^{-1} \leq Kn < 10$ (small $Re$)
- **Free-molecule regime:** $Kn \geq 10$ ($Re \rightarrow 0$)

![Figure 2. Knudsen number regimes and its limits on the gas modeling.](image)

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What Knudsen number regime do MEMS usually lie in? As an example, consider a cube of one micron with standard air flowing inside. The air temperature is 300K, and pressure 1atm. The cube contains about $2.45 \times 10^7$ molecules with an average molecular spacing of $3.4 \times 10^{-3} \mu m$. The ratio of this length to the effective molecular diameter of air ($4.19 \times 10^{-4} \mu m$) is about 8.1, which exceeds the dilute gas criteria of 7 (Bird 1994). The flow can be treated as dilute gas. The mean free path computed from equation (1.2) is 0.053μm. The $Kn$ would be 0.053 in such MEMS with characteristic length of 1μm. The flow is in the slip-flow regime. At lower pressure, the Knudsen number increases. For example, at a pressure of 0.1atm and other conditions unchanged, $Kn$ would be 0.53 and the flow is then in the continuum-transition regime. Therefore, it is reasonable that MEMS have $Kn$ in the range from 0.001 to 1.0 (Karniadakis and Beskok 2002). Over this $Kn$ range is the Nano technology. The flows in MEMS are in the slip-flow or transition regime, as shown in Figure 2.

**Molecular-based Models**

The molecular-based models recognize the particular structure of the gas as a myriad of discrete particles and ideally provide information on the position, velocity and state of every particle at all times. The particles may be molecules, atoms, ions and electrons. The mathematical model at this level is the Boltzmann equation. This has the fraction of particles in a given location and state as its single dependent variable. The independent variables for monatomic molecules are time and phase.
space that includes the three spatial coordinates and three components of molecular velocity. For diatomic or polyatomic molecules, the dimension of phase space increases with the number of internal degrees of freedom. Orientation adds an extra dimension for molecules that are not spherically symmetric. Clearly, the complexity of the approach increases dramatically as the dimension of phase space increases. The simplest problems are, for example, those for steady, one-dimensional flow of a simple monatomic gas. As shown in Figure 1, the molecular-based approach is either deterministic or statistical.

The most fundamental model among the molecular-based approaches is a deterministic model. The motion of the molecules is governed by the laws of classical mechanics. All simulation procedures are deterministic, except for the specification of the initial conditions. The well-known MD (molecular dynamics) simulation is a deterministic approach (see, for example, the early work of Alder and Wainwright 1957, 1958, and 1970). The simulation begins with a large number of particles; each assigned a random velocity corresponding to a Boltzmann distribution at the temperature of interest. The interaction between the particles is prescribed typically in the form of a two-body potential energy and the time evolution of the molecular positions is determined by integrating Newton’s equations of motion. Because MD is based on the most basic set of equations, it is valid in principle for any flow extent and any range of parameters. The method is straightforward to implement in principle but it requires immense computer resources to simulate a reasonable flow.

A serious limitation of MD simulations is the number of molecules $N$ that can
be realistically modeled in computing. Since the computation of the motion of any particular particle requires consideration of all other particles as potential collision partners, the amount of computing work required by MD is proportional to $N^2$. For example, a state-of-the-art supercomputer takes a few hours to handle around 100 thousand particles. The fastest parallel machine available can simulate about 10 million particles. MD simulations are highly inefficient for dilute gases when the molecular interactions are infrequent and their uses are restricted to flows of dense gases (Bird 1994).

An alternative to the deterministic molecular dynamics is the statistical approach where the goal is to compute the probability of finding a molecule at a particular position and state. If the appropriate conservation equation can be solved for the probability distribution, important statistical properties such as the number density, momentum and energy of the molecules within an element of volume can be computed from simple weighted averaging. In a practical problem, it is normally the average quantities that concern us rather than the details for every single molecule. The accuracy of computing average quantities, via the statistical approach, improves as the number of molecules in the sampled volume increases.

There have been two well-known statistical simulation approaches. The first one is the test particle Monte Carlo method, which has been introduced by Haviland and Lavin (1962). This method computes trajectories of a large number of test particles with initially assumed velocity distribution. A new distribution is then constructed from the history information of the test particles. The process is repeated
until changes in the distribution are negligible all over the flow field. The second is the direct simulation Monte Carlo (DSMC) method, which was primarily developed by Bird (1963; 1965a; 1976; 1978; 1994). Unlike the MD method, which is applicable only to dense gas flows, the DSMC method is suited for dilute gas flows where the average molecular spacing is an order of magnitude larger than the effective molecular diameter. It almost guarantees that all collisions between molecules are binary collisions, avoiding the complexity of modeling multiple encounters. DSMC is valid for all ranges of Knudsen number, although it becomes computationally expensive for $Kn < 0.1$. Fortunately, this is the continuum or slip-flow regime where the Navier-Stokes equations or Burnett equations can be used and will be briefly described in the next section. DSMC is therefore ideal for the transition regime.

DSMC is a random number strategy based directly on the physics of the individual molecular interactions. The idea is to track a large number of statistically representative particles, and to use their motions and interactions to modify their position and state. The primary approximation of DSMC is to uncouple the molecular motions and the intermolecular collisions over small time intervals. A significant advantage of this approximation is the amount of computation required is proportional to the number of molecules simulated $N$, in contrast to $N^2$ for MD simulations. In essence, particle motions are modeled deterministically while collisions are treated probabilistically, each simulated molecule representing a large number of actual molecules. On current state-of-the-art PC clusters, one can calculate flows with hundreds of millions of molecules by DSMC in about one month.
The DSMC computation is started from some initial condition and followed in small time steps that can be related to physical time. Collision pairs of molecule in a small computational cell in physical space are randomly selected based on a probability distribution after each computation time step. Complex physics such as radiation, chemical reactions, and mass species can be included in the simulations without the necessity of nonequilibrium thermodynamic assumptions that commonly afflict nonequilibrium continuum flow calculations. The DSMC technique is explicit and time marching, and therefore always produces unsteady flow simulations. For steady flows, DSMC simulation proceeds until a steady state is established within a desired accuracy. The macroscopic flow quantities are then determined by the time average of all cell-based quantities. For unsteady flows, ensemble averaging of many independent Monte Carlo simulations is carried out to obtain the final results within a prescribed statistical accuracy.

The discrete methods are approximated from the Boltzmann equation, where the Lattice-Gas Cellular Automata (LGCA) and Discrete Velocity (DV) are two types of the most popular models. There have been many models of these two types. The first model of LGCA is the HPP method (Hardy etc. 1973). LGCA is computationally more efficient than the DSMC method, but does not accurately simulate the physics of real gas flows (Bird 1994). This is because the technique limits particle motions to predetermined node locations. Particle interactions computed on a spatially fixed array of nodes conserve mass and momentum, but not energy, resulting in physically unrealistic gas simulations (Bird 1994; Wolf-Gladrow 2000). One early discrete
velocity model (DVM) was due to Broadwell (1964a; 1964b). The DV method replaces the Boltzmann equation by a set of nonlinear hyperbolic differential equations in velocity that is discretized on computational grids. The number of equations is equal to the number of discrete velocities, and the collision term involves a double summation over the velocity points. The solution of this set is a difficult task, and the accuracy to the approximation of the Boltzmann equation develops with a very large number of discrete velocities (>10^3). The challenges involved in solving the resulting set of equations have limited its applications to simple geometries and simple molecular flows.

### Continuum-based Models

In the continuum regime (\(Kn < 10^{-3}\), as shown in Figure 2), the mean free path of the gas molecules is much smaller than the characteristic length of the flow. The flow is collision dominated. *Traditional hydrodynamic equations* (THE) such as the Euler and Navier-Stokes equations serve as an appropriate model to describe the properties of a fluid in this regime and have been widely used in CFD. In the slip-flow regime (\(10^{-3} \leq Kn < 10^{-1}\)), deviations from the state of continuum are relatively small and the flow can still be governed by the Navier-Stokes equations (Schaaf and Chambre 1961). The slightly rarefied gas effects are modeled through the partial slip at the wall using the boundary conditions of velocity-slip and temperature-jump. The compressible Navier-Stokes equations with slip boundary conditions can barely lead to solutions of MEMS flows in slip-flow regime, especially with a \(Kn\) close to 0.1
The Navier-Stokes equations break down in the continuum-transition regime (\( Kn \geq 0.1 \)). As mentioned above, the molecular-based DSMC can be an alternative method. But DSMC, especially in the three-dimensional MEMS flows of such regime, is computationally very intensive both in terms of computing time and memory requirements, almost beyond what is currently available with a single-computer. Fortunately for the moderately rarefied effects, higher-order constitutive relations have been proposed for the viscous stress and heat flux. The equations with higher order terms are the Burnett equations, which are known as the generalized hydrodynamic equations (GHE) and will be briefly described in the following paragraphs.

Continuum constitutive relations for flows of dilute gas can be derived as a series Chapman-Enskog expansion of the Boltzmann equation with Knudsen number as a parameter. Retaining the first order approximation of this expansion leads to a linear constitutive relations in the Navier-Stokes equations; retaining the second order approximation leads to the nonlinear additional terms in second-order in the constitutive relations of Burnett equations. Burnett equations have been successfully applied to the hypersonic rarefied gas problems. Fiscko and Chapman (1988a; 1988b) have showed that the Burnett equations provide much more accurate numerical solutions than the Navier-Stokes equations for one-dimensional hypersonic shock structure in monatomic gases. In the application of many MEMS, the flows are in the continuum-transition regime. That is, the gas mean-free path is comparable to the characteristic length scale of the devices. As the Knudsen number increases, the flow
departs further and further from equilibrium and the second order Burnett terms become important. The application of Burnett equations to MEMS flows is one of the investigations conducted in this research (Liou and Fang 2001b).

The Burnett equations have a long and distorted development history. The difficulties in obtaining the Burnett solutions contributed to their rare uses until the work of Fiscko and Chapman in 1988. The Burnett equations have been a subject of considerable investigations in recent years. The complexity of the highly nonlinear viscous stress and heat flux terms is enormously challenging to analyze and to compute.

Table 1 shows a brief history of the Burnett equations (Agarwal et al. 1999). The Burnett equations were first derived by Burnett in 1935, referred to as the original Burnett equations. Then they were completed by Chapman (Chapman and Cowling 1970) in 1939 and by Wang Chang (Wang Chang and Uhlenbeck 1970) in 1948. The material derivatives in the original Burnett equations were replaced by spatial derivatives obtained from inviscid Euler equations. The alternative form of the original Burnett equations is referred to as the conventional Burnett equations, which have been the set of higher order constitutive relations studied during the past decades.

In the last decade Fiscko and Chapman (1988a; 1988b) and Zhong (1991) have applied the conventional Burnett equations to extend the numerical methods for continuum flow into the continuum-transition regime by incorporating additional linear and nonlinear viscous stress and heat flux terms in the Navier-Stokes equations.
In one of the earliest attempts to numerically solve the Burnett equations, Fiscko and Chapman (1988b) solved the hypersonic shock structure problems by relaxing an initial solution to steady state. The calculated normal shock structure is more accurate than the Navier-Stokes solutions at high Mach numbers. However, they also experienced numerical stability problems when the computational grids were made progressively finer. Zhong (1991) showed that the linear third order terms from the \textit{Super-Burnett} equations, which is a higher-order approximation beyond the conventional Burnett equations, could be added to stabilize the conventional Burnett equations, maintaining the second-order accuracy in the viscous stress and heat flux terms in the Burnett equations. This set of equations was named the \textit{augmented Burnett equations}. The coefficients of these linear third order terms were determined by carrying out a linearized stability analysis. The augmented Burnett equations did not present any stability problems when computing the hypersonic shock structure and hypersonic flows around blunt bodies. But attempts to simulate the flowfield for blunt body wakes and flat plate boundary layers with the augmented Burnett equations have not been entirely successful. It has been noted by Welder et al. (1993) that the linear stability analysis alone is not sufficient to explain the instability of Burnett equations with increasing $Kn$ as the analysis does not take into account many nonlinear terms that are present in the conventional Burnett equations. Comeaux et al. (1995) also assumed that this instability is attributed to the fact that the conventional Burnett equations can violate the second law of thermodynamics at high Knudsen numbers.
Table 1

Brief History of Burnett Equations (Agarwal et al. 1999)

<table>
<thead>
<tr>
<th>Equations</th>
<th>Author</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>Original Burnett Equations</em></td>
<td>Burnett (1935)</td>
<td>▪ Derived from the Boltzmann equation by considering the first three terms of the Chapman-Enskog expansion.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>▪ Appearance of the material derivatives in the second-order (Burnett) flux vectors.</td>
</tr>
<tr>
<td><em>Conventional Burnett Equations</em></td>
<td>Chapman (1939)</td>
<td>▪ Euler equations were used to express the material derivatives in terms of the spatial derivatives.</td>
</tr>
<tr>
<td><em>Conventional Burnett Equations</em></td>
<td>Fiscko and Chapman (1988)</td>
<td>▪ Problems with small wave length instability as the grids were refined.</td>
</tr>
<tr>
<td><em>Augmented Burnett Equations</em></td>
<td>Zhong (1991)</td>
<td>▪ Linearized third-order terms were added to stabilize the Burnett equations</td>
</tr>
<tr>
<td></td>
<td></td>
<td>▪ Not entirely successful for computing blunt body wakes and flat plate boundary layers.</td>
</tr>
<tr>
<td><em>Conventional Burnett Equations</em></td>
<td>Welder et al. (1993)</td>
<td>▪ Due to the nonlinear terms in the Burnett equations, linear stability analysis alone is not sufficient to explain the instability at high Knudsen numbers.</td>
</tr>
<tr>
<td><em>Conventional Burnett Equations</em></td>
<td>Comeaux et al. (1995)</td>
<td>▪ Burnett equations can violate the second law of thermodynamics at high Knudsen numbers.</td>
</tr>
<tr>
<td><em>BGK-Burnett Equations</em></td>
<td>Balakrishnan and Agarwal (1996)</td>
<td>▪ Nonlinear collision integral in the Boltzmann equation simplified by representing it with the Bhatnagar-Gross-Krook (BGK) model.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>▪ Material derivatives expressed in terms of the spatial derivatives using Navier-Stokes equations.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>▪ Linear stability analysis shows unconditional stability for all Knudsen numbers.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>▪ When the Euler equations are used to express the material derivatives, it guarantees unconditional stability for monatomic gases.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>▪ Entropy consistent (satisfy the Boltzmann’s H-theory) for a wide range of Knudsen numbers.</td>
</tr>
</tbody>
</table>

In order to overcome the difficulties associated with the conventional Burnett equations, Balakrishnan and Agarwal (1996, 1997) have developed *BGK-Burnett*
equations by using the first three terms in the Chapman-Enskog expansion. In the derivation, Euler equations were used to approximate the material derivatives in the first-order distribution function. Moments of the first-order distribution function with the collision invariant vector yield the Navier-Stokes equations. The Navier-Stokes equations were used to approximate the material derivatives in the second-order distributions function. The BGK-Burnett equations were obtained by take moments of this second-order distribution function with the collision invariant vector. This set of equations contains all the viscous stress and heat flux terms reported by Fiscko and Chapman (1988b) and additional terms similar to the super-Burnett terms. It has been shown that the BGK-Burnett equations are unconditionally stable for monatomic as well as polyatomic gases and do not violate the second-law of thermodynamics with these super-Burnett-like additional terms.

Zhong and Furumoto (1994) extended the two-dimensional augmented Burnett equations to axisymmetric geometries. They obtained numerical solutions for axisymmetric hypersonic flow past spherical blunt noses with Mach numbers and Knudsen numbers up to 21 and 0.2, respectively. Yun (1999) extended the numerical simulations to three-dimensional problems. All the results showed that the augmented Burnett solutions were in closer agreement with the DSMC results than Navier-Stokes solutions. Guo et al. (1999a; 1999b) applied the three-dimensional conventional Burnett equations to compute the transitional flow over a sphere and an elliptic cylinder and compared the results with the DSMC solutions. The Knudsen numbers were less than 0.01 and the differences between the solutions of the Burnett and the
Navier-Stokes equations were less than 2%.

Nearly all the applications of the various forms of the Burnett equations were for hypersonic flow around vehicles flying at high altitude. The solutions were normally in a better agreement with the DSMC predictions than the Navier-Stokes solutions. In this work, the conventional Burnett equations will be used to simulate the flows in microchannels, where there are rarefied gas effects.

Cost Effective Parallel Computing

The microfluidic simulations, either by solving the Burnett equations or by the DSMC molecular modeling, involve intensive numerical computing. Unsteady microflow simulations by DSMC in particular require state-of-the-art supercomputers with the highest possible performance. In order to be more tractable in the practical low-density, larger-scale flow simulation, the DSMC procedures should be parallelized and run on high performance computing systems. Parallel implementation of DSMC for high-speed rarefied gas applications has been reported in the literature (Boyd 1991; Wilmoth 1992; Wilmoth et al. 1992; Dietrich and Boyd 1994; Dietrich and Boyd 1995; LeBeau 1999). The computer platforms used include, for example, IBM SP-1, IBM SP-2, Cray C-90, and Cray T3E. These supercomputers cost millions of dollars to build, beyond the reach of all but a few of the most prestigious universities and laboratories. Fortunately, high performance computing on high performance computing clusters (HPCC) such as the Beowulf system (Sterling et al. 1999) is accelerating the development of CFD and other computational sciences and will be briefly described in the following paragraphs.
Development of HPCC

The history of the various supercomputers in the last 6 decades shows that the performance of the fastest computers have been increasing exponentially by two orders of magnitudes every decade on the average, as shown by the dash line in Figure 3. Most of the data presented in Figure 3 before 1994 is from the book of *Parallel Computing Works* (Fox et al. 1998). This tremendous rate of growth was accurately predicted by Moore’s law and is expected to continue in the future. But it does not hold for the growth rate of current parallel computer systems.

![Diagram showing historical trends of peak performance for sequential, parallel computers as well as high performance computing cluster (HPCC).](image-url)

Figure 3. Historical trends of peak performance for sequential, parallel computers as well as high performance computing cluster (HPCC).
Over the past 20 years, the performance of microcomputers has grown much faster relatively to that of highly specialized vector parallel machines. Ten years ago, the best vector processor outperformed the best microprocessor by a factor of 20,000. Today the difference is a factor of less than 10. The vector parallel computers use ECL (emitter-coupled logic) processors, which were specially built and offered at a very high price. The market for ECL was too small to drive rapid technological growth. In contrast, workstations and high-end PCs use microprocessors, which provide lower performance than ECL but a much lower price. In the early 1990s, the microprocessor-based highly parallel computers were introduced into the high-performance market by Thinking Machines, Kendall Square and Intel. These machines compensated for somewhat slower performance per processor by using more of the less expensive processors. Mainstream vendors like Cray, IBM, and Convex introduced their own such systems a few years later. Right now many of the high performance parallel systems in the TOP500 list, which ranks the performance of the most powerful supercomputer systems, use microprocessors. With the data taken from the Cray Inc. presentation (Cray Inc. 2003) and Intel website (Intel 2003), the comparison of peak performance for the fastest processors currently available is shown in Figure 4. The peak performance is counted in the 32-bit-floating-point operations per second (flop/s). It can be seen that the current fastest microprocessor, Intel Itanium2, is only about 3 times slower than the fastest vector processor used in the Cray X1 and ranks forth right after IBM P690 1.3. The second fastest processor NEC SX-6 used in the Earth Simulator, which is No.1 in the TOP500 list, is just
twice faster than Itanium2. In concluding, the advantage of the most expensive vector processors has decreased to a factor of 3.

Figure 4. Peak performances of the fastest processors currently available.

Also, the technology in fast Ethernet network has been rapidly developing with fast data transfer rate, low latency and high bandwidth. The improvement in microprocessors and the price/performance gained in the fast Ethernet network technology make HPCC affordable in the academic setting. A HPCC is a type of parallel or distributed processing system, which consists of a collection of interconnected stand-alone computers working together as a single, integrated computing resource. A computer node can be a single or multiprocessor system, such as PCs, workstations, or SMP (Symmetric Multiprocessors), with memory, I/O facilities, and an operating system. A HPCC generally refers to two or more computer-nodes connected together. The nodes can exist in a single cabinet or be
physically separated and connected via a *Local-Area Network* (LAN). An interconnected (LAN-based) cluster of computers appear as a single system to users and applications. Such a system can provide a cost-effective way to gain features and benefits (fast and reliable services) that have been found only on much more expensive centered-parallel machines such as nCube, CM5, Cray T3D, Cray T3E.

A typical architecture of a HPCC is shown in Figure 5. The network interface hardware acts as a communication processor and is responsible for transmitting and receiving packets of data between cluster nodes via a network/switch. Communication software offers a means of fast and reliable data communication among cluster nodes and to the outside world. Often, clusters with a special network/switch like Myrinet (1.28Gbps) use communication protocols such as active messages for fast communication among its nodes. They potentially bypass the operating system and thus remove the critical communication overheads providing direct user-level access to the network interface. The cluster nodes can work collectively, as an integrated computing resource, or they can operate as individual computers. The cluster middleware is responsible for offering an illusion of a united system image (single system image) and availability out of a collection on independent but interconnected computers. Programming environments can offer portable, efficient, and easy-to-use tools for development of applications. They include message passing libraries, debuggers, and profilers, such as MPI, MPE and PVM. It should not be forgotten that clusters could be used for the execution of sequential or parallel applications.
Figure 5. Typical architecture of HPCC (Buyya, R. 1999).

In the summer of 1994, the first HPCC system name Beowulf came to birth at NASA Goddard Space Flight Center (Sterling et al. 1999). It consisted of 16 66MHz Intel 80486 processors within a cost of $50K, which could compare to the comparable performance of Cray YMP with cost about 1 million dollars at that time, as shown in Figure 3. After that, the cost efficiency quickly spread through NASA and into academic and research communities. In 1997 ASCI Red was assembled at Sandia National Laboratories as the first stage Accelerated Strategic Computing Initiative (ASCI) plan to achieve a 100 TERAFOBP supercomputer system by 2004. ASCI Red consists of 9,216 Pentium Pro processors and was born as the fastest system (1.8 Tflop/s) (Tomkins 2003). In 1997 and 1998, the systems and services to achieve 1 gigaflop cost $3K to $3.5K. Today the cost is decreasing dramatically. For example, a typical Beowulf system shown in Figure 6 is going to be installed today. The system has 194 Pentium Xeon 2GHz CPUs with 100BaseT network speed. The peak performance is about 384 gigaflop with total cost about $210K. That is, the cost to
achieve 1 gigaflop has decreased to $550. Even if the efficiency is 40% considering the unbalance due to nonprofessional setting of network, the actual price/performance is about $1.4K per gigaflop. And the price/performance will continue to drop in the future.

Figure 6. Topology of a typical Beowulf system.

Just because of the main attractiveness mentioned previously, systems are built using affordable, low-cost, commodity hardware (such as Pentium PCs), fast LAN such as Myrinet, and standard software components such as UNIX, MPI, and PVM parallel programming environments. Scalable HPCC clusters, ranging from a cluster of PCs or workstations to SMP are rapidly becoming the standard platforms of
high-performance and large-scale computing. These systems are scalable, i.e., they can be tuned to available budget and computational needs. Cluster computing has been recognized as the wave of the future to solve large scientific and commercial problems.

In practical applications, there have been two main approaches for parallel programming:

1. The first approach is based on *implicit parallelism*. This approach is followed by parallel languages and parallelizing compilers. The user does not specify, and thus cannot control, the scheduling of calculations and/or the placement of data.

2. The second approach relies on *explicit parallelism*. In this approach, the programmer is responsible for most of the parallelization effort such as task decomposition, mapping tasks to processors, and the communication structure. This approach is based on the assumption that the user is often the best judge of how parallelism can be exploited for a particular application.

Explicit parallelism is usually much more efficient than parallel languages or compilers that use implicit parallelism. Parallel languages, such as SISAL (Feo et al. 1990) and PCN (Foster and Tuecke 1991) have found little favor with programmers. Parallel and their functions are still very limited. Parallelizing compilers are still limited to applications that exhibit regular parallelism, such as computations in loops. Parallelizing compilers have been used for some applications on multiprocessors and vector processors with shared-memory, but are unproven for distributed-memory machines. The difficulties are due to the NUMA (non-uniform memory access) in the
latter systems. Therefore, explicit parallelism is currently the only way on HPCC.

In explicit parallelism, parallel computing paradigms fall into two broad classes: functional decomposition and domain decomposition, as shown in Figure 7. These classes reflect how a problem is allocated to process. Functional decomposition divides a problem into several distinct tasks that may be executed in parallel; one field where this is popular today is that of Multidisciplinary Design Optimization. For CFD application, there are always many global variables inside each decomposed function. They will occupy a log of memory space. It is rarely used in CFD. On the other hand, domain decomposition distributes data across processes, with each process performing more or less the same operations on the data. In the application of CFD, domain decomposition splits a large problem into small problems and is warmly welcomed by coding programmers.

![Parallelization Diagram]

**Figure 7.** Parallel paradigms.
On the system of HPCC, the parallel programming paradigms can be classified into the well known ones: SPMD (Single Program Multiple Data), Task-Farming (or Master/Slave), Data Pipelining, Divide and Conquer, and Speculative Parallelism. SPMD is the most commonly used paradigm. Each process executes basically the same piece of code but on a different part of the data. This involves the splitting of application data among the available processors. SPMD applications can be very efficient if the data is well distributed by the processes and the system is homogeneous. If the processes present different workloads or capabilities, the paradigm requires the support of some load-balancing scheme able to adapt the data distribution layout during run-time execution. Therefore, there is still a lot of research work to do in the area of cost-effective high-performance parallel computing.

CEPCOM

A Cost Effective Computational Mast (CEPCOM) was assembled in the CFD laboratory at Western Michigan University. CEPCOM has been successfully used for the parallel simulation of microfluid flows in this dissertation work.

CEPCOM is a 23-node Beowulf-class cluster assembled in September 2001. Each node has two 1GHz Pentium III processors and 512MB RAM. The machines are connected via the fast-Ethernet network, which can support up to 100Mbps bandwidth for each node. A HP ProCurve Switch 4000M with a backplane speed of 3.8Gbps is used for the networking. The operating system is the Red Hat Linux 7.0. MPI library, mpich-1.2.2, is used for parallel programming in C/C++/Fortran77/Fortran90. The overall peak performance of CEPCOM is 46 Gflop/s, with total of 11.5GB RAM and
302GB hard drive space.

As shown in Figure 8 for the topology of CEPCOM, the system is implemented as a standalone network connected through a HP switch, with masked IP level 10.0.0.0. The client nodes have neither a gateway to the outside of the network nor any domain name service. That is, they work for and are controlled by only the server. The server node has a real Internet IP address, acting as the only access point to CEPCOM system from the outside world.

Figure 8. Topology of CEPCOM.

Figure 9 shows the LAN computing system. There can be two kinds of application on CEPCOM. One is high-throughput computing (HTC). In this case, many tasks (jobs, processes) can be run at the same time. Such applications do not need a communication between the tasks because they are independent. This is done through a job queuing system, PBS. The other is high-performance computing (HPC),
where the application needs a high-performance computing power to process a task in as short a time as possible. A problem is normally divided into subproblems such that it can be distributed and executed on different workstations with MPI.

![Diagram of CEPCOM LAN computing system]

**Figure 9.** LAN computing system of CEPCOM.

**Scope of the Dissertation**

The objective of this dissertation research is to numerically simulate and study the gas flow in microchannels by using the DSMC method and by solving the Burnett equations. The contents of this dissertation are briefly reviewed as follows.

Chapter II gives a brief derivation of the Boltzmann equation, which is the governing equation for dilute gas flows.

Chapter III describes the DSMC methodology and its basic kinetic theories. The main development of the DSMC method is introduced. The relationship between DSMC and the Boltzmann equation is discussed briefly. The Boltzmann equation can be derived from DSMC procedures, which shows that DSMC is as accurate as the Boltzmann equation. The chapter ends with the computational approximations of
DSMC.

Chapter IV presents the Burnett equations. First, the governing conservation equations are derived from the Boltzmann equation in detail. Then the derivation of the continuum constitutive relations of dilute gas flow, the detailed expressions of the conventional Burnett equations and augmented Burnett equations, and the slip-flow and temperature-jump boundary conditions are given.

Chapters V, VI, VII and VIII apply the DSMC method to simulate microchannel flows. Chapter V simulates supersonic microchannel flows, where the effects of $Kn$ on the heat transfer and flow field are studied. In Chapter VI, a new implicit boundary treatment is implemented for subsonic microchannel flows, and the numerical results are validated with analytical solutions. Chapter VII describes the parallelization of DSMC, the benchmark for parallel efficiency and the application to patterned microchannel flows. Chapter VIII develops a specified DSMC code to simulate forced chaotic flows.

Chapter IX solves the conventional Burnett equations to simulate the heat transfer and flowfield in microchannels.

Chapter X presents the summary, conclusions, and suggestions for future research.
CHAPTER II

BOLTZMANN EQUATION

Introduction

The Boltzmann equation is the bridge for analyzing the microfluid flows from both the molecular and continuum viewpoints. Several works have been done to derive the Boltzmann equation (Bird 1976, 1994; Cercignani 2000). In this chapter, the Boltzmann equation is briefly derived from basic kinetic theory, in order to correlate it to the DSMC method and understand further the accuracy of the Burnett equations in the later Chapters.

The Velocity Distribution Functions

In a classical sense, a gas flow would be completely described by listing the position, velocity, and internal state of every molecule at a particular instant. The number of molecules in a real gas is so large that such a description is inconceivable. An alternative is the statistical description in terms of probability distributions.

Consider a sample of gas that is homogeneous in physical space and contains $N$ identical molecules. A typical molecule has a velocity $\vec{c}$ and a position $\vec{r}$, with the velocity components $c_x$, $c_y$, and $c_z$ in the direction of the Cartesian axes $x$, $y$ and $z$. Just as $x$, $y$ and $z$ define a space called physical space, $c_x$, $c_y$, and $c_z$ define a velocity space. The physical space and the velocity space combine to form a phase space $(\vec{c}, \vec{r})$. Mathematically, the motion of every gas can be represented in the phase space.
It is assumed that the differential of the velocity space \((\bar{c})\) is expressed by 
\[ d\bar{c} = d\varepsilon_c d\varepsilon_c d\varepsilon_c, \]
and the differential of the physical space \((\bar{r})\) by 
\[ d\bar{r} = dx dy dz. \]
In a unit physical space \(d\bar{r}\) with a total number \(n\) of molecules, the number of molecules \(dn\) in a differential velocity space \(d\bar{c}\) is
\[ \frac{dn}{d\bar{c}} = nf(\bar{c}) \]  \hspace{1cm} (2.1)
Rearranging equation (2.1) leads to 
\[ f(\bar{c})d\bar{c} = (dn)/n. \]
That is, \(f(\bar{c})\) denotes the fraction of molecules with velocities between \(\bar{c}\) and \(\bar{c} + d\bar{c}\) in a unit physical space and is therefore called the velocity distribution function. If the velocity distribution function is applied to the whole physical space studied, the variables related to the physical position should be included and the corresponding velocity distribution function is \(f(\bar{c}, \bar{r})\). It is the velocity distribution function in the phase space \((\bar{c}, \bar{r})\) and the variables are usually omitted so that \(f(\bar{c}, \bar{r})\) becomes simply \(f\). Based on the definition, the total number of molecules \(N\) can be represented in a statistical way by integrating the product of number density \(n\) and the velocity distribution function \(f(\bar{c}, \bar{r})\) over all the possible molecular velocities and the physical space that the studied molecules occupy,
\[ N = \iiint n f(\bar{c}, \bar{r}) d\bar{c} d\bar{r} = \iiint nf d\bar{c} d\bar{r} \]  \hspace{1cm} (2.2)
In a unit physical space with its center located at \(\bar{r}\), the macroscopic quantity \(\bar{Q}\) of a quantity \(Q\) is defined as the average value of \(Q\) over all the molecules in the sample
and substituting for \( d_n \) from equation (2.1) yields

\[
\overline{Q}(\vec{r}) = \frac{1}{n} \int Q(\vec{r}) d_n
\]  

(2.3)

Omitting the functional statements, the general result is obtained as

\[
\overline{Q} = \int_{-\infty}^{\infty} Q f d\vec{c}.
\]  

(2.4)

Equation (2.4) establishes a moment of the distribution function and the macroscopic properties are referred to as moments of the distribution function. For example, the stream velocity may be written

\[
\vec{c} = \int_{-\infty}^{\infty} \vec{c} f d\vec{c}
\]  

(2.5)

The Boltzmann Equation

In statistical mechanics for gases, the conservation of the N-particle distribution function in 6N-dimensional phase space is described by the Liouville equation. The conservation of single particle distribution function, the Boltzmann equation, was introduced by Boltzmann early in 1872 (Bird 1994). The derivation will be briefly described. For clarity and simplicity, simple gases are assumed.

At a particular instant, the number of molecules in the phase space element \( d\vec{c} d\vec{r} \) is given by

\[
d N = n f d\vec{c} d\vec{r}
\]  

(2.6)

If the location and shape of the element does not vary with time, the rate of change of
the molecule number in the element is

\[ \frac{\partial}{\partial t} (nf) d\vec{c} d\vec{r} \]  (2.7)

Three processes contribute to the change in the molecule number within the phase space element \( d\vec{c} d\vec{r} \). As shown in Figure 10, they are:

I. **the convection of molecules across the face of \( d\vec{r} \) by the molecular velocity \( \vec{c} \),** shown as P I in Figure 10. The representation of the phase space element \( d\vec{c} d\vec{r} \) as separate volume elements, \( d\vec{c} \) and \( d\vec{r} \), in velocity and physical space, respectively, assumes that \( \vec{c} \) and \( \vec{r} \) are independent variables. \( \vec{c} \) is regarded as a constant within \( d\vec{r} \), and \( d\vec{c} \) is regarded as being located at the physical location defined by \( \vec{r} \).

II. **the molecule flux across the surface of \( d\vec{c} \) induced by the external force per unit mass \( \vec{F} \),** shown as P II. \( \vec{F} \) is regarded as a constant within \( d\vec{c} \). The effect of the acceleration \( \vec{F} \) on the molecules in \( d\vec{c} \) is analogous to the effect of the velocity \( \vec{c} \) on the molecules in \( d\vec{r} \).

III. **the scattering of molecules into and out of the phase space element \( d\vec{c} d\vec{r} \) as a result of internal molecular collisions,** shown as P III. With an assumption of dilute gases, the molecular collision is treated as an instantaneous event at a fixed location in physical space. This means that a collision causes a molecule to jump one velocity point to another one, remaining at the same point in physical space and time. Therefore, the collisions are represented as an affecting process only in the velocity space element \( d\vec{c} \). Another consequence of the dilute gas assumption is that all molecular collisions can be approximated as binary.
Figure 10. Molecular flux in a phase space element $d\bar{c} d\bar{\bar{r}}$.

In process I, the number density of class $\bar{c}$ molecules within $d\bar{\bar{r}}$ is $nf d \bar{c}$, and the net inflow of molecules of class $\bar{c}$ into the physical space element $d\bar{r}$ can be obtained as,

$$- \int_{S_r} (nf d \bar{c}) \bar{c} \cdot \bar{e}, dS_r$$  \hspace{1cm} (2.8)

where $S_r$ is the total area of the surface of $d\bar{\bar{r}}$, $dS_r$ a derivative element of this surface, and $\bar{e}_r$ the unit normal vector of the surface. Considering $nf$ and $\bar{c}$ are constant within $d\bar{\bar{r}}$, the Gauss' theorem enables the surface integral over $S_r$ of equation (2.8), yielding

$$- \bar{c} \cdot \frac{\partial (nf)}{\partial \bar{\bar{r}}} d\bar{c} d\bar{\bar{r}}$$  \hspace{1cm} (2.9)

Process II is analyzed in a similar fashion as in process I. The number density of class
molecules within \( d\vec{c} \) is \( n_f d\vec{r} \), and the net inflow of molecules of class \( \vec{r} \) into the velocity space element \( d\vec{c} \) can be modeled as,

\[
- \int_{S_c} (n_f d\vec{r}) \vec{F} \cdot \vec{e}_c dS_c
\]

(2.10)

where \( S_c \) is the total area of the surface of \( d\vec{c} \), \( dS_c \) an element of this surface, and \( \vec{e}_c \) the unit normal vector of the surface. Considering \( n_f \) and \( \vec{F} \) are constant within \( d\vec{c} \), equation (2.10) can be simplified as

\[
- \vec{F} \cdot \frac{\partial (n_f)}{\partial \vec{c}} d\vec{c} d\vec{r}
\]

(2.11)

In process III, binary collisions only cause molecular velocity to jump from one point in velocity space to another one. The increase rate of molecules resulted from molecular collisions inside the phase space element can be obtained through analyzing the collision rate for the direct and inverse collision processes, \((\vec{c}, \vec{c}_i) \leftrightarrow (\vec{c}^*, \vec{c}_i^*)\) (more details of the derivation refer to Bird 1994). Here it is considered with the collision of a molecule of class \( \vec{c} \) with one of class \( \vec{c}_i \) such that their post-collision velocities are \( \vec{c}^* \) and \( \vec{c}_i^* \), respectively. The direct collision processes mean that molecules scatter out of the phase space element \( d\vec{c} d\vec{r} \). The number of class \((\vec{c}, \vec{c}_i) \rightarrow (\vec{c}^*, \vec{c}_i^*)\) collision per unit time in an element of \( d\vec{c} \) is

\[
n^2 f f_i c, c^* d\Omega d\vec{c}_i d\vec{c} d\vec{r}
\]

(2.12)

Here \( c_i = |\vec{c} - \vec{c}_i| \) the magnitude of relative velocity of two collision molecules, \( \sigma \) the collision cross-section, and \( \Omega \) the solid angle with range from 0 to \( 4\pi \). Just as \( f \) is the value of the velocity distribution function at \( \vec{c} \), \( f_i \) denotes the value of \( f \) at \( \vec{c}_i \).
The inverse collision processes scatter molecules into class \( \bar{c} \). The number of class 
\((c, e_i) \leftarrow (c^*, e_i^*)\) collision per unit time in an element of \( d\bar{c} \) is

\[
n^2 f^* f^*_i c_\sigma d\omega d\bar{c} d\bar{c} d\bar{r}
\]  

(2.13)

where \( f^* \) and \( f^*_i \) denote the value of \( f \) at \( e^* \) and \( e^*_i \), respectively. The total rate of increase in the molecule of class \( \bar{c} \) in the phase space element \( d\bar{c} d\bar{r} \) as a result of collision is given by the integration of the difference between equation (2.13) and equation (2.12) over the complete cross-section for its collision with class \( \bar{c}_i \) molecules, followed by the integration of the class \( \bar{c}_i \) over all velocity space. The required expression for process III is obtained as

\[
\int_{-\infty}^\infty \int_0^{4\pi} n^2 (f^* f^*_i - f f_i) c_\sigma d\omega d\bar{c} d\bar{c} d\bar{r}
\]

(2.14)

The expression (2.7) for the total rate of increase of molecules of class \( \bar{c} \) due to all the three processes equals to the sum of expressions (2.9), (2.11) and (2.14). The Boltzmann equation for a simple dilute gas can be obtained by dividing the resulting equation by \( d\bar{c} d\bar{r} \)

\[
\frac{\partial}{\partial t} (nf) + \bar{c} \cdot \frac{\partial}{\partial \bar{r}} (nf) + \vec{F} \cdot \frac{\partial}{\partial \bar{c}} (nf) = \int_{-\infty}^{4\pi} \left\{ n^2 (f^* f^*_i - f f_i) c_\sigma d\omega d\bar{c} \right\}
\]

(2.15)
CHAPTER III

DSMC METHOD

Introduction

DSMC (Bird 1963; 1965; 1976; 1978; 1994) is a direct particle simulation method based on kinetic theory. The fundamental idea is to track thousands or millions of randomly selected, statistically representative particles, and to use their motions and interactions to modify their positions and states appropriately in time. Each simulated particle represents a number of real molecules. The primary approximation of DSMC is the uncoupling of the molecular motions and the intermolecular collisions over small time intervals that are less than the mean collision time. The DSMC computation is started from some initial conditions and followed in small time steps that can be related to physical time. Collision pairs of molecule in a small computational cell in physical space are randomly selected based on a probability distribution after each computation time step. Complex physics such as radiation, chemical reactions, and species concentrations can be included in the simulations without invoking nonequilibrium thermodynamic assumptions that commonly afflict nonequilibrium continuum flow calculations. The DSMC technique is explicit and time marching, and therefore can produce unsteady flow simulations. For steady flows, DSMC simulation proceeds until a stationary flow is established.
within a desired accuracy. The macroscopic flow quantities are then the time average of the cell-based values. For unsteady flows, ensemble averaging of many independent Monte Carlo simulations is carried out to obtain the final results within a prescribed statistical accuracy.

A significant advantage of DSMC is that the total computation required is proportional to the number of molecules simulated $N$, in contrast to $N^2$ for the MD simulations. In essence, particle motions are modeled deterministically while collisions are treated statistically. The backbone of DSMC follows directly from classical kinetic theory, and hence the applications of this method are subject to the same limitations as the theory. These limitations are the fundamental assumption of molecular chaos and dilute gases. DSMC has been shown to be accurate at the Boltzmann equation level for monatomic gases undergoing binary collisions (Bird 1970, 1994).

The statistical error of a DSMC solution is inversely proportional to the square root of the sample size $N$. A large sample size is needed to reduce the statistical error. The primary drawback of DSMC is the significant computer resources required for simulating a practical flow.

Bird (1963) first applied the DSMC method to a homogeneous gas relaxation problem, and then he applied DSMC to flows of the shock structure problem (Bird 1965b). The detailed principles of DSMC can be found in the book of *Molecular Gas Dynamics* (Bird 1976) and the recent edition *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Bird 1994).
Since its introduction, significant research has been performed and reported on improving the accuracy of the DSMC method as well as expanding its application to various fluid flow problems. Improved and more complex physical molecular models have also been developed for DSMC. The original hard sphere (HS) molecular model has been extended to the more realistic variable hard sphere (VHS) model (Bird 1981), variable soft sphere (VSS) model (Koura and Matsumoto 1991, 1992), and generalized hard sphere (GHS) model (Hash and Hassan, 1993; Hassan and Hash, 1993). The Borgnakke-Larsen (BL) phenomenological model (Borgnakke and Larsen 1975) was introduced in 1975 to handle inelastic binary collisions of polyatomic gases. The BL collision model accounts for the vibrational and rotational nonequilibrium and it has been widely used. In 1987, Bird proposed a radiation model for use in radiative nonequilibrium flows. This model was used successfully in predicting the radiative heating on the Aero-Assist Flight Experiment (AFE) vehicle (Moss et al. 1988). A model for dissociation-recombination interactions was introduced by Nanbu (1991). Boyd et al. (1992) proposed a vibrational relaxation method for use with the VHS model. Methods for ternary reactions, which involve triple collisions, were suggested even through the binary collision law prevails in most flow problems. Several collision-sampling techniques were also developed. These include the time counter (TC) method (Bird 1976) and the no time counter (NTC) method (Bird 1989).

The accuracy of the gas-surface interaction model has also been improved. The boundary condition models initially used by Bird and earlier researchers are

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simple and provide only an approximation to real gas-surface interactions. More advanced boundary conditions for DSMC calculations, such as the Maxwell model, Cercignani-Lampis (C-L) and Cercignani-Lampis-Lord (CCL) models, were summarized in the publications of Cercignani and Lampis (1971), Cercignani (1988), Lord (1991, 1992) and Collins and Knox (1994). DSMC has been combined with the Monotonic-Lagrangian-Grid (MLG) algorithm, allowing the grid to automatically adapt to the local number density of the flowfield (Oh et al. 1995). DSMC has also been improved with the information preservation (IP) method, effectively reducing the statistical scatter for low-speed flows (Fan and Shen 1998, 2001; Cai et al. 2000; Sun and Boyd 2002). All of the above efforts have improved the computational accuracy and versatility of DSMC. A summary of these works is listed in Table 2.

Table 2
Summary of significant research efforts on DSMC methodology

<table>
<thead>
<tr>
<th>DSMC Model</th>
<th>Author</th>
<th>Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>BL</td>
<td>Borgnakke et al.</td>
<td>1975</td>
</tr>
<tr>
<td>VHS</td>
<td>Bird</td>
<td>1981</td>
</tr>
<tr>
<td>Radiation</td>
<td>Bird; Moss et al.</td>
<td>1987; 1988</td>
</tr>
<tr>
<td>NTC</td>
<td>Bird</td>
<td>1989</td>
</tr>
<tr>
<td>Dissociation</td>
<td>Nanbu</td>
<td>1990</td>
</tr>
<tr>
<td>Vibrational Relaxation</td>
<td>Boyd</td>
<td>1991</td>
</tr>
<tr>
<td>VSS</td>
<td>Koura et al.</td>
<td>1991, 1992</td>
</tr>
<tr>
<td>GHS</td>
<td>Hash et al.</td>
<td>1993</td>
</tr>
<tr>
<td>Boundary conditions</td>
<td>Collins and Knox</td>
<td>1994</td>
</tr>
<tr>
<td>DSMC-MLG</td>
<td>Oh et al.</td>
<td>1995</td>
</tr>
<tr>
<td>DSMC-IP</td>
<td>Fan and Shen, Sun and Boyd</td>
<td>1998, 2002</td>
</tr>
</tbody>
</table>

The applications of DSMC have been reviewed by Oran et al (1998). In the
last 3 decades, DSMC has been primarily used in the simulations of hypersonic rarefied-gas flows. The results have been validated well with many experimental data and DSMC has been widely accepted as an important numerical method in rarefied-gas flows. DSMC has been used for different applications. Campbell (1991) used DSMC to investigate the plume/free stream interactions applicable to a rocket exhaust plume at high altitudes. Celenligil et al (1989) simulate the flow for blunt AFE configuration. Boyd et al (1992) studied the flow of small nitrogen nozzles and plumes using DSMC and compared the numerical results well with Navier-Stokes equations solutions and experimental data. Carlson and Wilmoth (1992) used the DSMC to solve the Type IV shock-interaction problem at a scramjet cowl lip. Drags on spheres at hypersonic speeds were calculated for flows in continuum-transition regime and compared to experimental data by Dogra et al. (1992). Celenligil and Moss (1992) used a three-dimensional version of DSMC to study a delta wing configuration. Good comparison with the data from wind-tunnel experiments was found in the aerodynamic properties for hypersonic transitional flows.

Basic Kinetic Theories for DSMC

Since DSMC is a statistical approach directly based on kinetic theory of molecule motions, a brief summary is given, in this session, of some related basic relations from the kinetic theory for dilute, monatomic gases. These relations provide the basis for the DSMC algorithm. A dilute gas is one in which the mean molecular spacing $\delta$ is about seven or more times the effective molecular diameter $d$. That is

$$\frac{\delta}{d} \geq 7$$  \hspace{1cm} (3.1)
Only a small fraction of space is occupied by the dilute molecules. Consequently, and such molecules can be assumed to be moving freely without the influence by the force field of molecules, and the binary molecular collisions are most likely to occur. The number of molecules per unit volume is called the number density of molecules, \( n \). The mean molecular spacing of molecules is inversely proportional to the number density and has a relations of

\[
\delta = n^{-1/3}
\]  

(3.2)

Assuming the molecules to be hard, elastic sphere with diameter \( d \), two molecules approaching each other collide when the distance between centers decreases to \( d \), as shown in Figure 11. The total collision cross-section, \( \sigma_t \), for such collisions between two hard sphere molecules is

\[
\sigma_t = \pi d^2
\]  

(3.3)

Figure 11. Binary collisions of hard-sphere molecules with diameter \( d \).

The collision cross-section may be interpreted as the area around a collision molecule.
into which the center of the incoming molecule cannot penetrate. For simple hard sphere molecules, $\sigma_T$ is constant as given by equation (3.3). For realistic molecule models, the value of $\sigma_T$ is a function of the relative speed $c$, between the molecules involved and must be obtained from experiment or from higher-order models.

In order to quantify the length and time scales of the macroscopic processes, it is necessary to establish the relationship for some important quantities of gases at the microscopic scale. The time scale of the macroscopic processes is the *mean collision time*, which is defined as the mean time between the successive collisions suffered by any particular molecule. The reciprocal of this quantity is more common in use and is called the *mean collision rate* or *collision frequency* $\nu$ per molecule. In order to specify it, we can fix our attention to a given molecule temporally, which is referred to as the test molecule with speed $\tilde{c}$, as shown in Figure 12. The velocities of the other molecules are distributed in an unspecified distribution function $f$. Consider those molecules of class $\tilde{c}$ with an assumed number density $\Delta n$. The velocity of the test molecule relative to the field molecules of class $\tilde{c}$ is $\tilde{c} = \tilde{c} - \bar{c}$. Then it could be approximated that, moving over a small time interval $\Delta t$ from time $t$, the test molecule would collide with any field molecule of class $\tilde{c}$ which has its center within the cylinder of volume $\sigma_T c, \Delta t$. The number of these molecules is $\Delta n \sigma_T c, \Delta t$, which is just the probability of a collision between the test molecule and a molecule of class $\tilde{c}$ in the time interval $\Delta t$. The collision rate with a class $\tilde{c}$ molecule is then $\Delta n \sigma_T c$. The mean collision rate for the particular test molecule is obtained by summing over all velocity classes and therefore over all values of $c$. That is,
Figure 12. Effective volume swept out by a test molecule over a small time interval.

\[ V = \frac{Y}{\tau} - \frac{\pi a^2 n c_r}{\tau} \]

and

\[ v = \bar{n}_a \bar{c_r} \]

A bar over a quantity or expression denotes the average value over all molecules in the sample. For molecules of hard sphere model, equation (3.5) becomes

\[ v = n \sigma c_r \]

and the mean collision time, \( t_c \), is

\[ t_c = \frac{1}{v} = \frac{1}{n \pi a^2 c_r} \]

The total collision rate per unit volume of gas is therefore given by

\[ N_c = \frac{1}{2} n v = \frac{1}{2} n^2 \sigma c_r \]
molecules.

The mean free path $\lambda$ is the average distance traveled by a given molecule between collisions in a frame of reference moving at the mean velocity of the flow stream. In other words, it is the value of the mean thermal velocity of the molecules divided by the mean collision frequency $\nu$, i.e.

$$\lambda = \frac{\nu}{\sqrt{\frac{2}{\pi m}} \sigma} = c'/\bar{n}$$

for molecules of the hard sphere model, the mean free path becomes

$$\lambda = \frac{1}{n \pi d^2}$$

The microscopic scales, such as mean collision time and mean free path of molecules, offer a chance to understand the macroscopic quantities of physical processes from a first principle point of view. In fluid dynamics, results are usually expressed in terms of macroscopic quantities such as pressure, density and temperature. Before establishing the relationships between the microscopic and macroscopic quantities, it is necessary to consider the properties of gas in equilibrium. A gas may be regarded as being in a state of equilibrium if it remains undisturbed for a time that is sufficiently long in comparison with the mean collision time. For a large gas sample where statistical fluctuations are negligible, there are no spatial or temporal gradients in the macroscopic quantities. In this state, the molecules have no preferred distribution in the velocity and are isotropic. The equilibrium velocity distribution function $f$, also known as the Maxwellian distribution function, can be derived in Cartesian coordinates by statistics (Bird 1994) as
where \( c' \) is the magnitude of thermal velocity, \( c' = (c'_x^2 + c'_y^2 + c'_z^2)^{1/2} \), and \( c_{mp} \) the most probable molecular thermal velocity as 

\[
c_{mp} = \sqrt{2RT}
\]  

In polar coordinates \((c', \theta, \phi)\), equation (3.11) becomes 

\[
f_{c'\theta \phi} = \frac{4c'^2}{\sqrt{\pi}c_{mp}} \exp\left[-\left(\frac{c'}{c_{mp}}\right)^2\right]
\]  

The average thermal velocity \( \overline{c'} \) can be obtained through the integration of the molecular thermal speed \( c' \) with its distribution function of equation (3.13) as 

\[
\overline{c'} = \frac{2}{\sqrt{\pi}} c_{mp}
\]  

For the hard sphere model, the average relative velocity \( \overline{c_r} \) of molecules undergoing binary collisions in an equilibrium state (equation 4.46 of Bird 1994) is 

\[
\overline{c_r} = \sqrt{2} \overline{c'} = \frac{2\sqrt{2}}{\sqrt{\pi}} c_{mp}
\]  

Derivation of the macroscopic variables can be found in Bird (1976, 1994). Here, some relevant expressions are listed for reference purpose. The density \( \rho \) is given as 

\[
\rho = nm
\]  

the specific kinetic energy associated with translational motion as, 

\[
e_a = \frac{1}{2} \overline{c'^2}
\]
the thermodynamic temperature as,

\[ T = \frac{2}{3R} e = \frac{2}{3R} e^{1/2} \]  

(3.18)

and the pressure as,

\[ p = \frac{1}{3} \rho e^{1/2} = n k T \]  

(3.19)

Using the Chapman-Enskog theory for transport properties, it may be obtained that the coefficient of kinetic viscosity \( \nu \) in a hard sphere gas is,

\[ \nu = \frac{5}{32} \pi e^{1/2} \lambda_0 \]  

(3.20)

and the coefficient of heat conduction \( K \) is

\[ K = \frac{15}{4} R \mu \]  

(3.21)

where

\[ \lambda_0 = \frac{1}{\sqrt{2\pi n d^2}} \]  

(3.22)

is the mean free path in an equilibrium gas of hard spheres.

Molecular Models for DSMC

The Lennard-Jones (L-J) Potential

It is usually assumed that the intermolecular force function includes molecular attraction at large distances and repulsion at small ones. The most well known mathematically convenient model, taking into account molecular attraction and repulsion as shown in Figure 13, is the Lennard-Jones (L-J) model with the force
field,

\[ F = 48 \frac{\varepsilon}{\delta} \left[ \frac{1}{2} \left( \frac{r}{\delta} \right)^7 - \left( \frac{r}{\delta} \right)^{13} \right] \]  

(3.23)

or with potential function,

\[ \phi = 4\varepsilon \left[ \left( \frac{r}{\delta} \right)^6 - \left( \frac{r}{\delta} \right)^{12} \right] \]  

(3.24)

where \( r \) is the distance between the two molecules, \( \varepsilon \) is the minimum potential value, and \( \delta \) a characteristic length scale, the distance at which the potential function changes its sign. The deflection angle, \( \chi \), is defined as

\[ \chi = \pi - 2W \left[ 1 - (WW_i)^2 - \frac{1}{6} \left( \frac{WW_i}{W_0} \right)^{12} + \frac{1}{3} \left( \frac{WW_i}{W_0} \right)^{11/2} \right] dW \]  

(3.25)
the reduced mass of the two collision molecules and $b$ an impact parameter of the projected distance between the pre-collision/post-collision velocities of the two collision molecules.

In MD simulations, the L-J model is commonly used to model intermolecular interactions between dense gases or liquid molecules and between fluid and solid molecules. In the statistical simulation, the dependence of $\chi$ on two parameter $W_0$ and $W_0^*$ necessitate the use of interpolation tables for computing the maximum impact parameters and deflection angles. In order to find the deflection angle of $\chi$ for a pair of collision molecules, it is necessary to determine the value $b_{\text{max}}^*$ from the interpolation tables at a specified deflection angle cut-off, sample $b^*$ and find $\chi$ using the tables again. Because of the high computational cost of this process, as well as difficulties in determining the mean free path, the L-J potential is typically applied only to homogeneous relaxation cases and simple one-dimensional problems.

The Inverse Power Law (IPL) Potential

A more suitable model of high-temperature flows, where intermolecular repulsion prevails, is the inverse power law (IPL) model,

$$ F = \frac{\kappa}{r^\delta} \quad \text{(3.26)} $$

or

\[ F = \frac{\kappa}{r^\delta} \]

where $W = \frac{b^*}{r^*}$, $W_0 = b^* \left( \frac{c}{24} \right)^{1/12}$, $W_0^* = b^* \left( \frac{c}{12} \right)^{1/6}$, $b^* = \frac{b}{\delta}$, $r^* = \frac{r}{\delta}$, $c = \frac{m_1 c_1^2}{2 \epsilon}$, with $m$, the reduced mass of the two collision molecules.
where $\eta$ is the power determining the "hardness" of particles, $\kappa$ a constant, and $r$ the molecular separation distance. The deflection angle $\chi$ is,

$$
\chi = \pi - 2 \int_{W_0}^{\infty} \left[ \left( 1 - W^2 - \frac{2}{(\eta - 1)} \right) \left( W/W_0 \right)^{\eta-1} \right]^{1/2} dW
$$

(3.28)

where $W_0 = b(m_c^2 / \kappa)^{1/\eta-1}$, $b$ is an impact parameter as defined in the L-J model, and the dimensionless $W_0$ is the positive root of the equation,

$$
1 - W^2 - \frac{2}{(\eta - 1)} (W/W_0)^{\eta-1} = 0
$$

(3.29)

Note that $\chi$ is a function of the dimensionless impact parameter $W_0$ only. This single parameter dependence of the deflection angle is the basic reason for the usefulness of the IPL model. For any finite value of $\eta$, the force field extends to infinity, and the total cross-section is,

$$
\sigma_T = \int_0^{\pi} \sigma \, d\Omega = \int_0^{\pi} \int_{W_0}^{\infty} \left\{ \kappa / (m_c^2) \right\}^{2(\eta-1)} W_0 \, dW_0 \, d\Omega = \infty
$$

(3.30)

To use the IPL model in DSMC simulation, it is necessary to limit $\sigma_T$. This can be achieved by specifying either a deflection angle cut-off or a maximum impact parameter value. In most cases, the latter is chosen. Since $\chi$ is a function of $W_0$, the deflection angle cut-off may be applied through the specification of a maximum value $W_{0,m}$ of $W_0$. And equation (3.30) can be integrated to,

$$
\sigma_T = \pi W_{0,m}^2 \left\{ \kappa / (m_c^2) \right\}^{2(\eta-1)}
$$

(3.31)
The Hard Sphere (HS) Model

The hard sphere (HS) model is a special case of the IPL model with \( \eta = \infty \). Another special case is the Maxwell model with \( \eta = 5 \). The value of \( \eta \) for the HS model and the Maxwell model are generally accepted as the limiting cases for "hard" and "soft" molecules, respectively. For a real monatomic molecule, the effective value of \( \eta \) is about 10.

For the HS model, it has been shown that the total cross section \( \sigma_T \) is constant, as given in equation (3.3). The molecular scattering is isotropic so that the post-collision velocity is uniform in solid angle. The HS model is simple and easy to incorporate into DSMC procedures. However, its primary deficiency is that this scattering law is not realistic. For a real gas, \( \sigma_T \) is a strong function of \( c_r \) and the relative translational energy \( E_r \), given by

\[
E_r = \frac{1}{2} m_c c_r^2
\]

In the HS model, the viscosity coefficient \( \mu \) is proportional to \( T^{0.5} \), instead of the more realistic \( T^{0.75} \) variation (Bird 1994).

The Variable Hard Sphere (VHS) Model

The variable hard sphere (VHS) model was introduced by Bird (1981) to correct the primary deficiency of the HS model. In the VHS model, the molecule is a hard sphere with a diameter \( d \) that is a function of \( c_r \). Generally the function can be obtained based on a simple inverse power law \( \alpha \), so that
\[ d = d_{\text{ref}} \left( \frac{c_{t, \text{ref}}}{c_t} \right)^\alpha \]  

(3.32)

where the subscript "\text{ref}" denotes the reference values at the reference temperature \( T_{\text{ref}} \), and \( \alpha = \frac{2}{(\eta - 1)} \).

For the VHS model, \( \sigma_t \) is expressed in terms of reference conditions

\[ \sigma_t = \sigma_{\text{ref}} \left( \frac{c_t^2}{c_{t, \text{ref}}^2} \right)^\alpha \]  

(3.33)

For an equilibrium gas, \( c_t \) is related to temperature by

\[ c_t^2 = \frac{2(2 - \alpha)kT}{m_t} \]  

(3.34)

Combining equation (3.33) and equation (3.34) yields an expression for \( \sigma_t \), appropriate for an equilibrium gas, as

\[ \sigma_t = \sigma_{\text{ref}} \left( \frac{m_t c_t^2}{2(2 - \alpha)kT_{\text{ref}}} \right)^\alpha \]  

(3.35)

The VHS model leads to a power law temperature dependence of the coefficient of viscosity by

\[ \mu \propto T^\omega \]  

(3.36)

where \( \omega = 0.5 + \alpha \), and the deflection angle

\[ \chi = 2 \cos^{-1} \left( \frac{b}{d} \right) \]  

(3.37)

The VHS model is currently the most popular one for DSMC simulations, because of its simplicity and its good approximation to real intermolecular potential.

In a DSMC simulation, \( \sigma_{\text{ref}} \), \( T_{\text{ref}} \) and \( \alpha \) are known parameters. For the molecular collisions, \( c_t \) is determined and the value of \( \sigma_t \) is calculated using equations (3.35).
Typical values of $\alpha$ and $d_{ref}$ are given in Table 3 (Bird 1994).

Table 3

Typical values of $\alpha$ and $d_{ref}$ for VHS molecules at 273K

<table>
<thead>
<tr>
<th>Gas</th>
<th>Symbol</th>
<th>$\alpha$</th>
<th>$d_{ref} \times 10^{-8}$ m</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>H$_2$</td>
<td>0.17</td>
<td>2.92</td>
</tr>
<tr>
<td>Helium</td>
<td>He</td>
<td>0.16</td>
<td>2.33</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>N$_2$</td>
<td>0.24</td>
<td>4.17</td>
</tr>
<tr>
<td>Oxygen</td>
<td>O$_2$</td>
<td>0.27</td>
<td>4.07</td>
</tr>
<tr>
<td>Argon</td>
<td>Ar</td>
<td>0.31</td>
<td>4.17</td>
</tr>
<tr>
<td>Carbon dioxide</td>
<td>CO$_2$</td>
<td>0.43</td>
<td>5.62</td>
</tr>
</tbody>
</table>

The Variable Soft Sphere (VSS) Model

Both the HS and VHS models have the same impact parameter $b = d \cos(\chi/2)$. The effective diameter $d$ is invariant for the HS model, but is an energy-dependent variable for the VHS model. Both models obey the isotropic scattering law and do not correctly predict the diffusion in flows of real gases, especially of gas mixtures. To overcome this deficiency, the variable soft sphere (VSS) model (Koura and Matsumoto 1991, 1992) was introduced to take into account the anisotropic scattering of real gases, where the molecular diameter varies in the same way as the VHS model, but there is a deflection exponent, $\beta$, in the relation for $b$ such that

$$b = d \cos^\beta(\chi/2)$$  \hspace{1cm} (3.38)

This cosine exponent $\beta$ and the diameter $d$ are determined such that the viscosity and diffusion coefficient are consistent with the IPL potential. For the VHS model, $\beta$ is 1. This model is called variable soft sphere because $\chi_{vss}$ is smaller than $\chi_{vhs}$,
which can be obtained from $\beta > 1$ and $\cos(\chi_{\text{VHS}}/2) = \cos^\beta(\chi_{\text{VSS}}/2)$. The VSS total collision cross section can be expressed as

$$\sigma_{\text{T,VSS}} = \frac{1}{S} \sigma_{\text{T,VHS}} \tag{3.39}$$

where $S$ is the softness coefficient given by

$$S = 6\beta /[(\beta + 1)(\beta + 2)] \tag{3.40}$$

The values of the cosine exponent $\beta$ and softness coefficient $S$ for a large variety of molecular species are compiled in Koura and Matsumoto (1991). In addition, the corresponding viscosity and diffusion cross-section for the VSS model are also given in the reference. It was found that the VSS model is preferable to the VHS model in flows of gas mixtures where molecular diffusion is important.

The Generalized Hard Sphere (GHS) Model

The generalized hard sphere (GHS) model (Hash and Hassan 1993) is an extension of the VHS and VSS models. It bears the same relationship to the L-J class of potential as the conventional VHS and VSS models bear to the IPL potential. The scattering distribution is that of the hard or soft sphere, but the variation of the total cross section as a function of the relative translational energy mimics that of the corresponding attractive-repulsive potential. It is implemented through the parameters that describe the intermolecular potentials of the form of equation (3.32), and can therefore make use of the existing database that has been built up from the measured transport properties of real gases.
The Borgnakke-Larson (BL) Phenomenological Model

There have been molecular models proposed for inelastic collision. The most successful and widely used is the Borgnakke-Larson (BL) phenomenological model (Borgnakke and Larson 1975), applicable for binary collisions in a mixture of polyatomic gases. This model allows molecules to have continuous internal energy modes. The exchange of energy among translational, rotational and vibrational modes is accounted for in distribution of post-collision velocity for the molecules involved. The BL model was also extended to include the repulsive force described in the GHS model.

DSMC Methodology

The procedures involved in applying DSMC to steady or unsteady flow problems are presented in Figure 14 (Bird 1976). Execution of the method requires the physical domain to be divided into a grid of computational cells. The cells provide geometric boundaries and volumes required to sample macroscopic properties. It is also used as a room where only molecules located within the same cell, at a given time, are allowed for collision. The cell dimensions, $\Delta x$, must be such that the change in flow properties is small (Bird 1976). This requires that $\Delta x$ must be much smaller than the characteristic length of the geometry, or less than $\lambda/3$ in general. It is also important that the selection of a time step, $\Delta t$, should be less than the molecular mean collision time. Simulation results are independent of a time step increment as long as this requirement and the cell-size requirement on the gradient

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solutions are satisfied.

Figure 14. DSMC flow chart (Bird 1976).

Like a continuum CFD calculation, a DSMC simulation proceeds from a set of prescribed initial condition. The molecules are initially distributed in the computational domain. These simulated molecules, each representing a large number of real gas molecules, are assigned random velocities, usually based on the equilibrium distribution. Physically correct molecular sizes and weights are always used in the calculation of gas properties. The particle positions, velocities, collision cross sections, and boundary conditions determine the subsequent evolution of the
system. The solution may be sensitive to the particular choice of initial, boundary, and input conditions (Oran et al. 1998).

The core of the DSMC algorithm consists of four primary processes: move the particles, index and cross-reference the particles, simulate collisions, and sample the flow field. These procedures are uncoupled during each time step.

In the first process, the simulated representative molecules are moved for a convection time step of $\Delta t_i$. This molecule motion is modeled deterministically. This process enforces the boundary conditions and samples macroscopic properties along solid surfaces. Modeling molecule-surface interactions requires applying the conservation laws to individual molecules instead of using the velocity distribution function. Such treatment of the boundary conditions allows DSMC to be extended to include physical effects such as chemical reactions, catalytic walls, radiation effects, three-body collisions, and ionized flows, without major modifications in the basic procedure. Other boundaries, such as the inflow/outflow boundaries or plane of symmetry, are also imposed during this step.

The second DSMC process involves indexing and tracking particles. A scheme for molecular referencing is the prerequisite for the next two steps: modeling collisions and sampling the flow field. Efficient indexing and tracking are keys to practical DSMC applications for large-scale processing.

The molecular collision process is modeled statistically, which is different from deterministic simulation methods such as MD. Only particles within a given computational cell are considered to be possible collision partners. With each cell, a
representative set of collisions is taken in account, and collision pairs are selected randomly. The post-collision velocities are determined before particles are allowed to move for the next time step $\Delta t_d$. Uncoupling the molecular motions and the intermolecular collision requires that $\Delta t_d$ be smaller than the mean collision time. There are several collision-sampling methods that have been used successfully. The currently preferred model is the no-time-counter (NTC) technique (Bird 1994) used in conjunction with the sub-cell technique (Bird 1986). The sub-cell method calculates local collision rates based on the individual cell but restricts possible collision pairs to sub-cells. The procedure improves accuracy by ensuring that collisions occur only between near neighbors.

The final process is sampling the macroscopic flow properties. The spatial coordinates and velocity components of molecules in a particular cell are used to calculate macroscopic quantities at the geometric center of the cell. The other steps of the DSMC procedure do not depend on the sampling process. The computational time can be reduced through sampling the flow properties every nth time step.

The DSMC procedures are explicit and time marching, and therefore always produce unsteady flow simulation. For a steady flow problem, a DSMC simulation proceeds until steady flow is established at a sufficiently large time $t_L$, and the desired steady result is a time average of all values sampled after reaching a steady state. To simulate an unsteady flow, an ensemble of many independent computations may be assembled and averaged to obtain final results with an acceptable statistical accuracy. An ensemble average, the instantaneous average over area or volume elements of an
arbitrarily large group of similar systems, is commonly used to present unsteady DSMC results.

Binary Collisions

In a collision, two scattering angles, $\chi$ and $\varepsilon$, are defined for DSMC simulation. $\chi$ is the deflection angle as defined previously, the angle between the pre-collision relative velocity and the post-collision relative velocity. $\varepsilon$ is the azimuthal impact angle measured between the collision plane and some reference plane. For hard sphere collisions (HS and VHS), both of the scattering angles, $\chi$ and $\varepsilon$, are uniformly distributed. In terms of the molecule diameter $d$ and the impact parameter $b$, we can have $b/d = \cos(\chi/2)$. For VSS collisions, a parameter $\beta$ is used to characterize the anisotropy of the deflection angle as

$$\left(\frac{b}{d}\right)^{\beta \chi} = \cos\left(\frac{\chi}{2}\right)$$

The parameters must be used for computing the post-collision relative velocity $\vec{c}_i^*$ as a function of the pre-collision relative velocity $\vec{c}_i$ and the post-collision relative speed $c_i^*$. For elastic collision, $c_i^*$ is simply the magnitude of $c_i$.

$$c_i = |\vec{c}_i - \vec{c}_2|$$

while for inelastic collisions it may be different. The procedure for computing $\vec{c}_i^*$ is as follows.

First, the azimuthal impact angle $\varepsilon$ is computed using a random fraction $R_{\varepsilon}$ as
\[ e = 2 \pi R_{t_1}, \]  
(3.43)

Second, the deflection angle \( \chi \) is computed using another random fraction \( R_{t_2} \),

\[ \cos \chi = 2 R_{t_2}^\beta - 1 \]  
(3.44)

\[ \sin \chi = \sqrt{1 - \cos^2 \chi} \]  
(3.45)

Next, a set of Cartesian coordinates \((x', y', z')\) is introduced with \( x' \) in the direction of \( \vec{c}_r \). The vector \( \vec{g}_i \) representing \( \vec{c}_r \) in this coordinate system \((x', y', z')\) is

\[ \vec{g}_i = (c, \cos \chi, c, \sin \chi \cos \epsilon, c, \sin \chi \sin \epsilon) \]  
(3.46)

The pre-collision relative velocity \( \vec{c}_r \) has components of \((u_r, v_r, w_r)\) in the original Cartesian coordinates \((x, y, z)\). The direction cosines of \( x' \) are \((u / c_r, v / c_r, w / c_r)\) in the original coordinates. Since the orientation of the reference plane is arbitrary, the \( y' \)-axis may be chosen to be normal to the \( x \)-axis. The direction cosines of \( y' \) are then \((0, v_r (v_r^2 + w_r^2)^{-1/2}, -v_r (v_r^2 + w_r^2)^{-1/2})\). Those of \( z' \) are \((((v_r^2 + w_r^2)^{1/2}) / c_r, -u_r v_r (v_r^2 + w_r^2)^{-1/2} / c_r, -u_r (v_r^2 + w_r^2)^{-1/2} / c_r)\). So, the coordinate transformation from \((x', y', z')\) to \((x, y, z)\) is a second order tensor \( \vec{g}_T \) of

\[
\vec{g}_T = \begin{bmatrix}
-u_r / c_r & v_r / c_r & w_r / c_r \\
0 & w_r (v_r^2 + w_r^2)^{-1/2} & -v_r (v_r^2 + w_r^2)^{-1/2} \\
(v_r^2 + w_r^2)^{1/2} / c_r & -u_r v_r (v_r^2 + w_r^2)^{-1/2} / c_r & -u_r (v_r^2 + w_r^2)^{-1/2} / c_r
\end{bmatrix}
\]  
(3.47)

The components of \( \vec{c}_r \) in the original coordinate system can be obtained through the product of vector \( \vec{g}_i \) with the tensor \( \vec{g}_T \), as

\[ \vec{c}_r = \vec{g}_i \cdot \vec{g}_T \]  
(3.48)

and the required expressions of \( \vec{c}_r \) are
\[ u_r' = \cos \chi u_r + \sin \chi \cos \varepsilon (v_r^2 + w_r^2)^{1/2} \] (3.49a)

\[ v_r' = \cos \chi v_r + \sin \chi (c_r, w_r \cos \varepsilon - u_r, v_r \sin \varepsilon) / (v_r^2 + w_r^2)^{1/2} \] (3.49b)

\[ w_r' = \cos \chi w_r - \sin \chi (c_r, v_r \cos \varepsilon - u_r, w_r \sin \varepsilon) / (v_r^2 + w_r^2)^{1/2} \] (3.49c)

From the conservations of momentum and energy, the post-collision velocities of the two collision molecules can be obtained as

\[ \tilde{c}_1' = \tilde{c}_m + \frac{m_2}{m_1 + m_2} \tilde{c}_r' \] (3.50a)

\[ \tilde{c}_2' = \tilde{c}_m - \frac{m_1}{m_1 + m_2} \tilde{c}_r' \] (3.50b)

where \( \tilde{c}_m \) is the velocity of the center of mass of the pair of collision molecules given by

\[ \tilde{c}_m = \frac{m_1 \tilde{c}_1 + m_2 \tilde{c}_2}{m_1 + m_2} \] (3.51)

Collision Sampling Techniques

Several collision-sampling techniques are discussed in Bird (1994). In this section, two of the most popular techniques, the time counter (TC) and the no time counter (NTC) sampling, are outlined. Both use acceptance-rejection statistics described by Bird (1976) to select the collision partners. The acceptance-rejection technique uses random numbers to determine whether a randomly selected pair of molecules will interact. The details of this technique will be described in Appendix A.

The probability of collision between two molecules in a homogeneous gas is proportional to the product of their relative speed \( c_r \) and total collision cross-section.
\( \sigma_T \). Equation (3.8) for the non-equilibrium collision rate in a homogeneous gas could be used to establish the number \( N_c \Delta t_d \) of collisions in each cell at each time step \( \Delta t_d \), and this number could be computed. The mean value of the product of \( c_r \) and \( \sigma_T \) is calculated for each cell, and the maximum value could also be recorded. The collision pairs could then be chosen by the acceptance-rejection method, with the probability, \( P \), of a particular pair being given by the ratio of their product of \( c_r \) and \( \sigma_T \) to the maximum product.

\[
P = \frac{\sigma_T c_r}{(\sigma_T c_r)_{\text{max}}} \tag{3.52}
\]

The TC technique assigns an incremental time \( \delta t \) to each collision. For HS and VHS molecules, \( \delta t \) is given by

\[
\delta t = \frac{2}{N_m \sigma_T c_r} \tag{3.53}
\]

where \( N_m \) is the number of simulated molecules in a cell. Sufficient collisions are simulated in each cell for the sum of all \( \delta t \) to equal to the convection time step \( \Delta t_d \).

The TC technique is very efficient. Its computational cost is directly proportional to \( N_c \). It has been found that TC technique predicts correct collision rates for moderate nonequilibrium flows. However, for flows with extreme nonequilibrium regions, such as in a very strong shock front, it gives inaccurate collision rate (Bird 1989). The TC technique allows the acceptance of unlikely collision pairs, resulting in an incorrect incremental time \( \delta t \). This problem was corrected by the NTC technique. In NTC method, the procedures are similar to those in the TC technique, except that the
summation of collision incremental time $\delta t$ is replaced by the summation of the number of collision pairs until it reaches the number of allowed collisions, $N_{cp}$, which is given by

$$N_{cp} = \frac{N_{m} \bar{N}_{m} S_{m} (\sigma_{i} c_{r})_{max} \Delta t_{d}}{2 V_{c}}$$

(3.54)

where $S_{m}$ is the number of real molecules a simulated molecule represents, and $V_{c}$ the cell volume. The computational cost of the NTC method remains directly proportional to $N_{m}$. It is the most widely used collision-sampling technique for DSMC and is also used in the present work.

Sub-Cell Schemes

Primitive implementations of the DSMC method choose the collision partners from any location in the same flow field cell. The DSMC method has been used successfully on a variety of problems as long as the fundamental constraints have been adhered to. However, in the mid-80's, Meiburg (1986) questioned the validity of the method, claiming that by allowing molecules from opposite sides of a cell to collide that DSMC could not support a rotational component within the cell. In response to the claim, Bird introduced the concept of sub-cells. In this scheme sub-cells are created by further sub-dividing a flow field cell and sorting molecules within that cell into the sub-cells. The standard collision methodology was then modified such that candidate collision pairs are formed at random from within the same sub-cell if possible. This reduces the separation distance between collision pairs,
effectively increasing the spatial resolution of the simulation at minimal additional computational cost.

In widely distributed code like Bird's G2/A3 software (Bird 1992), sub-cells were a fixed element of the flow field grid. In the case of the G2/A3 software, the sub-cell resolution was the same for all flow field cells in a given region, and the sub-cell resolution was specified as a preprocessing input and held static during the simulation. This required that the user specify the ratio of real-to-simulated molecules such that not only were the cells adequately populated with molecules, but also that the sub-cells were adequately populated as well.

The issue is not statistical representation, but rather the ability to even form a collision pair from within a sub-cell. If excessive sub-cell resolution is used with insufficient population of molecules, then it becomes more likely that there will be less than two molecules in a given sub-cell. Intelligent searching of the other sub-cells can add an additional layer of complexity and logic to the collision algorithm. This issue becomes even more acute for three-dimensional problems. If sub-cells are to be employed in a three-dimensional case, where each direction is bisected, there will be a total of $2^3$ sub-cells per cell. This would require the flow field cell to be populated with 16 molecules in order to populate each sub-cell with at least two molecules per cell on average. However, this is a best-case scenario, and often a sub-cell will have fewer than two molecules in it if only the absolute minimum average is maintained. This would require the implementation of an even more complex search algorithm than would be needed in a two-dimensional case.
As an alternative, Bird (2000) has devised transient-adaptive sub-cells. Transient-adaptive sub-cells attempt to minimize the under populated sub-cell issue, by dynamically determining the sub-cell resolution for each flow field cell based on the number of molecules in the cell. Here the sub-cell resolution to be targeted such that there are as many sub-cell as molecules. Dynamic sub-cells provide obvious advantages over static sub-cells, in terms of both usability and efficiency. However, the design of an appropriate search methodology to locate a second collision partner is still a relevant issue since on average there are fewer than two molecule in a sub-cell.

The static or transient-adaptive sub-cell scheme cannot guarantee that a sub-cell would have less than two molecules in it on occasion. LeBeau et al (2003) proposed a strategy termed virtual sub-cells. It simply involves picking the first collision partner at random, and then locating the nearest other molecule in the flow field cell as the second partner. But it introduces a $N^2$-like search algorithm to the procedure and takes additional computational cost. Only in case that the molecule number $N$ should be controlled and kept small in each flow field cell, the virtual sub-cell scheme is computationally competitive with the true sub-cell methods.

Gas-Surface Interactions

Only two theoretical models of molecular gas-surface interaction, specular and diffuse reflections shown in Figure 15, are typically used in DSMC applications. These two models were originally proposed by Maxwell in 1879 (Bird 1994). Boundary conditions are directly applied to individual molecules interacting with a specific surface.
Figure 15. Specular and diffuse reflection models for gas-surface interactions.

For the specular reflection model, the gas-surface interaction is treated as perfectly elastic. Also the surface is smooth, as an ideal mirror, and the incident molecule is reflected such that its velocity component normal to the surface is reversed, while the parallel component is conserved. This type of interaction is perfectly elastic and does not represent real molecule gas-surface interactions. It is used primarily for boundaries where the conservation of the number of molecules is required and for lines of symmetry. When using the specular reflection model, the viscous and thermal boundary layers adjacent to the boundaries are absent.

For the diffuse reflection model, the molecular gas-surface interface is not smooth. The velocity components of the reflected molecules are distributed according to an equilibrium distribution applied to half of a solid angle. The equilibrium distribution is based on a reflected temperature, $T_r$, which is not necessarily the same as the wall temperature $T_w$. The thermal accommodation coefficient $a_T$, defined as

$$a_T = (q_i - q_r)/(q_i - q_w)$$

may be used to control the extent of the thermal energy recovered by the reflected
molecules. In equation (3.55), \( q_i \) and \( q_r \) represent the incident and reflected energy fluxes, respectively, while \( q_w \) is the energy flux that would be carried away in diffuse reflection with \( T_r = T_w \). The accommodation coefficient \( a_T \) ranges from zero for no accommodation to one for complete thermal accommodation. For real gas, \( a_T \) is in between these two values and must be determined experimentally. For interactions at temperatures on the order of standard temperature, the fully diffuse reflection model with complete accommodation, i.e., \( T_r = T_w \), provides solutions that are in good agreement with experimental data. The thermal accommodation coefficient is significantly less than one for interaction of gases with carefully clean surface. Despite a great deal of research, no significant improvement from molecule-surface modeling has been obtained, mostly due to the lack of experimental validation of existing models.

Relationship to Boltzmann Equation

The general form of the Boltzmann equation for a simple dilute gas, equation (2.15) described in Chapter 2, defines the relationship between the velocity distribution function and its dependent variables. It is the governing equation for the entire transition regime of interest in this study. The Boltzmann equation is derived from the underlying fundamental principles of classical kinetic theory, and consequently is restricted to dilute gas flows in molecular chaos.

The DSMC method, on the other hand, is derived from the same first principles as the Boltzmann equation, but not from the equation itself. Due to its ties
to classical kinetic theory, the DSMC method is subjected to the same restrictions of
dilute gas and molecular chaos. Unlike the Boltzmann equation, however, the DSMC
method does not require the existence of inverse collisions that are dictated by
symmetry considerations of binary dynamics. This allows application of the method
to some complex phenomena, such as ternary chemical reactions, that are inaccessible
to the Boltzmann equation.

A derivation of the Boltzmann equation from DSMC procedures based on the
TC collision technique was presented by Bird (1976). A similar derivation for hard
sphere molecules based on the NTC collision technique is now presented.

The left hand side of equation (2.15) states that the quantity $n_f$ remains
constant in phase space in the absent of collisions if one moves along with a group of
molecules in a Lagrangian manner. Analogically, the DSMC procedures trace the
paths of simulated molecules in phase space, and the processes are consistent with the
Boltzmann formulation. Any discrepancy between DSMC and the Boltzmann would
be from the collision term on the right hand side. The collision term conventionally
comprises the gain and loss terms of integral. The latter represents the rate of
scattering by collision out of the phase space element $d\vec{r}d\vec{v}$ per unit volume of this
element. This rate may be derived from the DSMC procedures by the following
argument.

The spatial cell in the simulated flow may be treated as the element $d\vec{r}$ of
physical space, and the set of $N_m$ molecules in the cell defines the velocity
distribution function $f$. The number of molecules of class $\bar{c}$ within the cell at time $t$
is \( n f \, d\vec{c} \, d\vec{r} \), or \( N_m f \, d\vec{c} \). Now consider a collision between a molecule of this class and one of class \( \vec{c}_i \). The probability to find a molecule in class \( \vec{c}_i \) is \( f_i \, d\vec{c}_i \), with \( f_i \) being of \( f \) at velocity \( \vec{c}_i \), and the collision rate for such collisions is

\[
\nu = \frac{(N_m f \, d\vec{c})(f_i \, d\vec{c}_i)}{\Delta t} \tag{3.56}
\]

For HS molecules, the increment of time \( \Delta t \) contributed by such a collision to a counter for class \( \vec{c} \) molecules is given from equation (3.6) by

\[
\Delta t = \frac{1}{n \sigma_r c_i} \tag{3.57}
\]

and substituting equation (3.57) into equation (3.56) yields to

\[
\nu = n^2 \sigma_r c_i f f_i \, d\vec{c}_i \, d\vec{c} \, d\vec{r} \tag{3.58}
\]

Finally, the rate of molecules per unit volume scattering out of class \( \vec{c} \), i.e., the loss term, is obtained by substituting \( \sigma_r \) from its definition, integrating class \( \vec{c}_i \) in equation (3.58) over velocity space, and dividing by \( d\vec{c} \, d\vec{r} \). The resulting expression

\[
\int \int d^3 c \int d\vec{c} (ff_i c_i \sigma d\vec{s} \, d\vec{c}_i)
\]

is identical to the loss term of the Boltzmann equation. The gain term in this expression can be derived in the same way as that for the loss term through the existence of inverse collisions for the simple monatomic gas models. Note that the DSMC method selects collision partners and replaces their pre-collision velocity components by appropriate post-collision values. Therefore, the correct gain term is automatically obtained without requiring the existence of inverse collision. This holds irrespective of the existence of inverse collisions and DSMC is less restrictive than...
the Boltzmann equation.

Since the procedures of the DSMC technique are consistent with the Boltzmann formulation, the results of DSMC provide an accurate solution to this equation as long as the computational approximations are kept within allowable bounds.

Computational Approximations and Input Data

Two distinct types of errors are associated with a DSMC simulation. The first type is in result of the computational approximations inherent to the method. These include errors due to the finite cell sizes in physical space; the finite size of the time step; the ratio of actual to simulated molecules; and various aspects of how boundary conditions are implemented. The second type of error is the result of uncertainties or inadequacies in the physical model input parameters. These include uncertainties about the type of species modeled, their interaction cross-sections, and other aspects of boundary conditions and interactions.

When the cell size in physical space is too big, macroscopic gradients are typically underpredicted. For accurate DSMC calculations, cell dimensions must be smaller than \( \lambda \) in each spatial direction. Another computational approximation involves the time interval over which molecular motions and collisions are uncoupled. The effects of the time step are negligible if the time step \( \Delta t \) is smaller than the mean collision time of molecules. DSMC procedures are not subject to a stability criterion such as the Courant-Friedrichs-Lewy (CFL) condition of continuum
CFD. Disturbances propagate at sound or shock speed throughout the DSMC computational domain, even though the ratio of spatial cell size to time step may be a smaller value.

Large values of the ratio, $S_m$, of the actual to simulated molecules are typical in most applications, and lead to unacceptably small statistical scatter levels in a single independent computation. To reduce the scatter to acceptable levels, the results of a large ensemble average are needed. Typical values of $S_m$ used in calculations may range from $10^9$ to $10^{18}$ for a three-dimensional computation. In problems involving chemical reactions or thermal radiation, large value of $S_m$ is particularly problematic. Important physical effects, caused by only a few molecules, may not be simulated properly. In these cases, special remedies, such as those proposed by Bird (1994) and Boyd (1996) are required.

The errors associated with various models and input data are not easily summarized as those inherent to the method itself. Input data may consist of the type of molecular gas-surface interactions or the total collision cross-sections.

Any numerical result obtained in gas dynamics, whether by DSMC or a continuum CFD method, depends on an accurate treatment of surface interactions. The DSMC method relies on gas-surface interaction models that are simple, fast, and accurate for a wide range of engineering problems. The primary types of molecular-surface interactions used in DSMC have been described previously. The thermal accommodation coefficient $a_T$ is an input parameter, which is usually determined experimentally. Another input data is the total collision cross-section $\sigma_T$, which is the
equivalent of the chemical reaction in continuum CFD. The models for $\sigma_r$ may range from the simplest hard-sphere model to complex models for inelastic collisions that account for vibrational and rotational nonequilibrium (Borgnakke and Larsen 1975). The HS model is sometimes adequate for idealized monotonic gas computations but not for real gases. The VHS model (Bird 1992) corrects for the primary deficiency in the hard-sphere model, namely an inaccurate representation of the total collision cross section, while retaining simplicity of implementation. The VSS model (Koura and Matsumoto 1991, 1992) further refines the VHS model by improving postcollision scattering dynamics. The GHS model (Hash and Hassan 1993) extends the VHS model to allow relaxation of internal models.
CHAPTER IV

BURNETT EQUATIONS

Introduction

At the microscopic level, dilute gases are considered to be particles that constantly and randomly move around and collide with one and the other. The general governing equation for flows at the microscopic level is the Boltzmann equation. Analytical solutions to the Boltzmann equation exist only for a few simple problems. Attempts to numerically solve Boltzmann equation have difficulties handling the collision integral term. Furthermore, without further development it is not apparent how the Boltzmann equation relates to the earlier Navier-Stokes equations from the continuum theory of gas dynamics.

The task of the kinetic theory of gases is to derive macroscopic properties of the gas in terms of microscopic characteristics of the molecules. The macroscopic equations in the continuum approach are the conservation equations of mass, momentum and energy, which can be derived as the moment equations of the Boltzmann equation. However, these conservation equations do not form a complete set of equations and constitutive relations for transport phenomena (viscous stress and heat flux) are needed to close the conservation equations. This chapter presents the constitutive relations derived by the Chapman-Enskog theory as approximate...
solutions of the Boltzmann equation for flows in the continuum transition regime. More extensive presentations of the kinetic theory of gases can be found in the books by Kennard (1938), by Chapman and Cowling (1970), by Wang Chang and Uhlenbeck (1970). Only a monatomic gas is discussed since the viscous stress and heat flux in a gas are caused by translational nonequilibrium effect.

General Conservation Equations

The velocity distribution function $f$ in the Boltzmann equation is the fraction of particles in a unit volume, which depends on time, the three components of molecular velocity, and the three components of molecular position.

$$f = f(c_i, x_i, t)$$

(4.1)

The physical interpretation of the velocity distribution function is that it gives the probability of finding a molecule at a given velocity at a given point at a certain time. From the velocity distribution function all desired macroscopic properties of the gas may be obtained by multiplying the distribution function by a certain quantity and then integrating over all velocity space, a process known as taking moments of the velocity distribution function. For example, density as a function of space and time is obtained by multiplying molecular mass and the velocity distribution function and then integrating. Hence one obtains the macroscopic quantities such as density, momentum, and energy from the velocity distribution function by

$$\rho = \rho(x_i, t) = \int_{-\infty}^{\infty} mnf \, d\bar{e} = \rho m$$

(4.2)

$$\rho u_i = \rho(x_i, t)u_i(x_i, t) = \int_{-\infty}^{\infty} mnc_i f \, d\bar{e}$$

(4.3)
\[\varepsilon = \int_{-\infty}^{\infty} \frac{1}{2} m (c_x^2 + c_y^2 + c_z^2) f \, d\mathbf{\vec{c}}\]  \hspace{1cm} (4.4)

where \(d\mathbf{\vec{c}} = d\mathbf{c} \, d\mathbf{c}_x \, d\mathbf{c}_y \, d\mathbf{c}_z\) is the differential element in the velocity space. Boltzmann (1872) also formulated the H-theorem, which states that a gas in equilibrium exhibits the property of detailed balance, namely that for equilibrium gases every molecular collision has a corresponding inverse collision. A direct consequence of the H-theorem is the Maxwellian velocity distribution of a gas in translational equilibrium, which was given in equation (3.11).

The quantity \(Q\) relates to a single molecule and is either a constant or a function of the molecular velocity. The multiplication of the Boltzmann equation (2.15) by \(Q\) yields

\[\frac{\partial}{\partial t} (nf) + \vec{Q} \cdot \frac{\partial}{\partial \mathbf{c}} (nf) + Q \vec{F} \cdot \frac{\partial}{\partial \mathbf{c}} (nf) = Q \int_{-\infty}^{\infty} n^2 (f^* f_i^* - ff_i) c_i \sigma d \Omega \, d\mathbf{\vec{c}}_i\]  \hspace{1cm} (4.5)

Through taking \(Q\) inside the derivative in equation (4.5) and integrating over the velocity space with the definition of a macroscopic quantity \(\overline{Q} = \int_{\mathbf{c}} Q \, d\mathbf{\vec{c}}\) of equation (2.4), equation (4.5) can be simplified to the so-called transfer equation or the equation of change as

\[\frac{\partial}{\partial t} (n\overline{Q}) + \nabla \cdot (n\overline{Q} + n\vec{F}) + n \overline{Q} \cdot \frac{\partial \overline{Q}}{\partial \mathbf{c}} = \Delta [Q]\]  \hspace{1cm} (4.6)

where the right hand side term \(\Delta [Q]\) is the collision integral as

\[\Delta [Q] = \int_{-\infty}^{\infty} n^2 Q (f^* f_i^* - ff_i) c_i \sigma d \Omega \, d\mathbf{\vec{c}}_i\]  \hspace{1cm} (4.7a)

Two symmetries are associated with the collision term. The first symmetry is between
the collision partners and means that $\Delta[Q]$ is unchanged if $\bar{c}$ and $\bar{c}_i$ are interchanged and $Q$ which represents a value at $\bar{c}$ is interchanged with the value of $Q_i$ at $\bar{c}_i$.

Similarly, $\bar{c}^*$ and $Q^*$ may be interchanged with $\bar{c}_i^*$ and $Q_i^*$. The second symmetry is based on the existence of inverse collisions and is between the pre-collision and post-collision velocities. It enables $Q$ and $Q^*$ or $Q_i$ and $Q_i^*$ to be interchanged, as long as $\bar{c}$, $\bar{c}_i$, $f$ and $f_i$ are interchanged with $\bar{c}^*$, $\bar{c}_i^*$, $f^*$ and $f_i^*$. These two symmetries lead to an alternative form to $\Delta[Q]$ of

$$\Delta[Q] = \frac{1}{2} \int \int \int n^2 (Q' + Q_i' - Q - Q_i) f_i f \bar{c} \sigma d \Omega d \bar{c}_i d \bar{c}$$  \hspace{1cm} (4.7b)$$

Equations (4.6) and (4.7b) are called the $Q$-equation. If the quantity $Q$ is either the mass $m$, the momentum $m\bar{c}$, or energy $\frac{1}{2}mc^2$ of a molecule, the conservation of these quantities in collisions requires that $Q' + Q_i' - Q - Q_i = 0$, and the collision integral is zero in the three equations for those quantities. The averages on the left hand side of the $Q$-equation can be expressed in terms of the macroscopic gas properties. The three equations are the conservation equations of gas dynamics.

The conservation equation for mass is obtained by setting $Q = m$ in the $Q$-equation, to give

$$\frac{\partial}{\partial t} (nm) + \nabla \cdot (nm\bar{c}) = 0$$  \hspace{1cm} (4.8)$$

or

$$\frac{\partial}{\partial t} (\rho) + \nabla \cdot (\rho \bar{c}_0) = 0$$  \hspace{1cm} (4.9)$$
The conservation equation for momentum is obtained by setting $Q = m\ddot{c}$ in the $Q$-equation. This is a vector equation

$$\frac{\partial}{\partial t}(\rho \vec{c}) + \nabla \cdot (\rho \vec{c} \vec{c}) = \rho \vec{F} = 0 \quad (4.10)$$

With $\vec{c} = \vec{c}_0 + \vec{c}'$ and $\vec{c} \vec{c} = \vec{c}_0 \vec{c}_0 + \vec{c}' \vec{c}'$, equation (4.10) can be written

$$\frac{\partial}{\partial t}(\rho \vec{c}_0) + \nabla \cdot (\rho \vec{c}_0 \vec{c}_0) = -\nabla \cdot (\rho \vec{c}' \vec{c}') + \rho \vec{F} \quad (4.11)$$

In equation (4.10), $\rho \vec{c}' \vec{c}'$ is a tensor of second-order, called the pressure tensor $\vec{p}$. That is,

$$\vec{p} = \rho \vec{c}' \vec{c}' \quad (4.12)$$

From equation (4.12), it can be seen that the pressure tensor represents the momentum $m \vec{c}'$ transport by the thermal motion. The pressure tensor can be decomposed to the scalar pressure $p$ and viscous stress tensor $\vec{t}$ by

$$\rho \vec{c}' \vec{c}' = \delta_{ij} p + \vec{t} \quad (4.13)$$

where $\delta_{ij}$ is the Kronecker delta such that $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$, and the scalar pressure $p$ is defined as the average of the three normal components of the pressure tensor; i.e.

$$p = \frac{1}{3} \rho (\vec{u}'^2 + \vec{v}'^2 + \vec{w}'^2) = \frac{1}{3} \rho \vec{c}'^2 \quad (4.14)$$

Substituting equation (4.13) into equation (4.11) yields

$$\frac{\partial}{\partial t}(\rho \vec{c}_0) + \nabla \cdot (\rho \vec{c}_0 \vec{c}_0) = -\nabla p + \nabla \cdot \vec{t} + \rho \vec{F} \quad (4.15)$$

$Q$ may be set equal to $\frac{1}{2} m \dot{c}^2$ in the $Q$-equation to give the conservation equation for
energy as

\[ \frac{\partial}{\partial t} \left( \frac{1}{2} \rho \vec{c}^2 \right) + \nabla \cdot \left( \frac{1}{2} \rho \vec{c} \vec{c}' \right) - \rho \vec{c}_0 \cdot \vec{F} = 0 \]  

(4.16)

With \( \vec{c}^2 = c_o^2 + c'c' \) and \( \vec{c}c' = c_o^2 \vec{c}' + \vec{c}_0(c_o^2 + c'^2) + 2(\vec{c}_0 \cdot \vec{c}') \vec{c}' \), equation (4.16) can be written

\[ \frac{\partial}{\partial t} \left[ \frac{1}{2} \rho (c_o^2 + c'^2) \right] + \nabla \cdot \left[ \frac{1}{2} \rho \vec{c}_0 (c_o^2 + c'^2) \right] = -\nabla \cdot \left[ \frac{1}{2} \rho \vec{c}' \right] - \nabla \cdot [\rho (\vec{c}_0 \cdot \vec{c}') \vec{c}'] + \rho \vec{c}_0 \cdot \vec{F} \]  

(4.17)

The second term in the right hand side of equation (4.17) \( \rho (\vec{c}_0 \cdot \vec{c}') \vec{c}' \) can be transformed as

\[ \rho (\vec{c}_0 \cdot \vec{c}') \vec{c}' = c_o \cdot \rho \vec{c}' \vec{c}' = c_o \cdot \vec{D} = c_o \cdot (\delta_v \rho - \vec{r}) \]  

(4.18)

Substituting equation (4.18) into equation (4.17) yields

\[ \frac{\partial}{\partial t} \left[ \frac{1}{2} \rho (c_o^2 + c'^2) \right] + \nabla \cdot \left[ \frac{1}{2} \rho \vec{c}_0 (c_o^2 + c'^2) \right] = 
-\nabla \cdot \left[ \frac{1}{2} \rho \vec{c}' \right] - \nabla \cdot (\rho \vec{c}_0) + \nabla \cdot (\vec{c}_0 \cdot \vec{r}) + \rho \vec{c}_0 \cdot \vec{F} \]  

(4.19)

In equation (4.19), \( \frac{1}{2} \rho \vec{c}' \vec{c}' \) is a vector representing molecular thermal energy \( e = \gamma \frac{1}{2} m \vec{c}'^2 \) transport by thermal motion and is called the heat flux vector \( \vec{q} \) for monatomic gas. That is,

\[ \vec{q} = \frac{1}{2} \rho \vec{c}' \vec{c}' \]  

(4.20)

And \( \nabla \cdot (\vec{c}_0 \cdot \vec{r}) \) is the viscous dissipation function \( \Phi \); i.e.

\[ \Phi = \nabla \cdot (\vec{c}_0 \cdot \vec{r}) \]  

(4.21)

With substituting of equations (4.20) and (4.21) and setting the molecular total
internal energy \( E_t \),

\[
E_t = \frac{1}{2} c_0^2 + \frac{1}{2} \epsilon^2
\]  

(4.22)

the final result for macroscopic quantities of equation (4.19) may then be

\[
\frac{\partial}{\partial t}(\rho E_t) + \nabla \cdot (\rho \ddot{c}_t E_t) = \nabla \cdot \ddot{q} - \nabla \cdot (\rho \ddot{c}_t \rho) + \Phi + \rho \ddot{c}_t \cdot \ddot{F} \]  

(4.23)

Equations (4.9), (4.15) and (4.23) are the conservation equations of Boltzmann equation in conservative form for mass, momentum and translational energy, respectively. They are expressed by tensor, and can be expanded to the form in Cartesian coordinates as

\[
\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x_j}(\rho u_j) = 0 \tag{4.24}
\]

\[
\frac{\partial}{\partial t}(\rho u_j) + \frac{\partial}{\partial x_j}(\rho u_j u_j + \delta_{ij} p) = \frac{\partial \tau_{ij}}{\partial x_j} + \rho F_i \tag{4.25}
\]

\[
\frac{\partial}{\partial t}(\rho E_t) + \frac{\partial}{\partial x_j}(\rho u_j (E_t + \frac{p}{\rho}) = \frac{\partial}{\partial x_j} (q_j + u_j \tau_{ij}) + \rho u_j F_j \tag{4.26}
\]

where \( i = 1,2,3 \) and \( j = 1,2,3 \). In equation (4.26), the conservation equations are generally valid for gas flow under any Knudsen number. However, they do not form a closed set of equations. The Five equations in equations (4.24-26) plus necessary equations of state are not sufficient to determine the five flow field variables \( (\rho, u_i, \text{and } e) \), because of the additional five unknown dependent variables in the viscous stress terms \( \tau_{ij} \) and the additional three unknown dependent variables in the heat flux terms \( q_j \). The relations of \( \tau_{ij} \) and \( q_j \) terms with the quantities \( \rho, u_i, e \) and their spatial gradients are termed the constitutive relations. To close the conservation
equations, the constitutive relations for a gas near equilibrium can be derived by the Chapman-Enskog theory in solving the Boltzmann equation.

Chapman-Enskog Theory

The Chapman-Enskog theory (Chapman and Cowling 1970) provides a solution of the Boltzmann equation for gas flows near thermodynamic equilibrium, where the velocity distribution function $f$ is perturbed by a small amount from the equilibrium Maxwellian form. It is assumed that the expansion of the distribution function for small values of Knudsen number as follows

$$f = f^{(0)} + f^{(1)} + f^{(2)} + f^{(3)} + \cdots$$

$$= f_0(1 + Kn\phi_1 + Kn^2\phi_2 + \cdots + Kn^n\phi_n) + o(Kn^{n+1})$$

(4.27)

where the $n$ represents the order of accuracy with respect to $Kn$. The first term $f^{(0)}$ is the Maxwellian distribution function $f_0$, which is the zeroth order of $Kn$.

From the distribution function above, the constitutive relations for a gas flow of small $Kn$ can be derived as approximate solutions of the Boltzmann equation. Substituting equation (4.27) into equation (4.13) and equation (4.20) leads to the following constitutive relations

$$\begin{align*}
\tau_y &= \tau_y^{(0)} + \tau_y^{(1)} + \tau_y^{(2)} + \tau_y^{(3)} + \cdots + \tau_y^{(n)} + o(Kn^{n+1}) \\
q_j &= q_j^{(0)} + q_j^{(1)} + q_j^{(2)} + q_j^{(3)} + \cdots + q_j^{(n)} + o(Kn^{n+1})
\end{align*}$$

(4.28)

The derivations of this procedure are beyond the present scope. Details may be found in the book of *The Mathematical Theory of Nonuniform Gases* (Chapman and Cowling 1970).

The zeroth order approximation ($n = 0$) corresponds to equilibrium flows that
are described by the Euler equation, i.e.,

\[
\begin{align*}
\tau_y^{(0)} &= 0 \\
q_j^{(0)} &= 0
\end{align*}
\]  \hspace{1cm} (4.29)

As \( Kn \) increases, a flow departs from thermodynamic equilibrium, and more and more higher order terms in equation (4.28) become significant. When a flow departs slightly from equilibrium (\( Kn < 0.1 \)) and it is still in the slip-flow regime as described in Figure 2, the first-order accuracy of equation (4.28) is valid. Only the first two terms in equation (4.28) are needed and they correspond to the well-known Navier-Stokes equations. As \( Kn \) becomes larger, we need to retain the first three terms to keep the second-order accuracy and obtain the Burnett equations. Similarly, the third-order solutions are the super-Burnett equations; and so on. The constitutive equations of the \( n \)th order approximation are

\[
\begin{align*}
\tau_y &\approx \tau_y^{(1)} + \tau_y^{(2)} + \ldots + \tau_y^{(n)} \\
q_j &\approx q_j^{(0)} + q_j^{(1)} + \ldots + q_j^{(n)}
\end{align*}
\]  \hspace{1cm} (4.30)

where the superscript \( n \) denotes the order of accuracy with respect to \( Kn \), with \( n = 1 \) for the Navier-Stokes equations, \( n = 2 \) the conventional Burnett equations, and \( n = 3 \) the super Burnett equations; and so on. The detailed expressions for \( \tau_y^{(n)} \) and \( q_j^{(n)} \) are given in the following section.

Constitutive Relations

The First Order Terms of \( \tau_y^{(1)} \) and \( q_j^{(1)} \)

The general expressions for \( \tau_y^{(1)} \) and \( q_j^{(1)} \) are as in the Navier-Stokes equations
\[
\begin{align*}
\tau^{(1)}_{ij} &= 2\mu(D_{ij} - \frac{1}{3}D_{\alpha\alpha} \delta_{ij}) \\
n_j^{(1)} &= K \frac{\partial T}{\partial \chi_j}
\end{align*}
\] (4.31)

where

\[
D_{ij} = \frac{1}{2}(\frac{\partial u_i}{\partial \chi_j} + \frac{\partial u_j}{\partial \chi_i})
\] (4.32)

and \(D_{\alpha\alpha} = D_{11} + D_{22} + D_{33}\). In three-dimensional Cartesian coordinates, the first order constitutive relations can be expressed as

\[
\begin{align*}
\tau_{xx}^{(1)} &= 2\mu u_x - \frac{2}{3}\mu(u_x + v_y + w_z) \\
\tau_{xy}^{(1)} &= 2\mu v_y - \frac{2}{3}\mu(u_x + v_y + w_z) \\
\tau_{xz}^{(1)} &= 2\mu w_z - \frac{2}{3}\mu(u_x + v_y + w_z) \\
\tau_{yx}^{(1)} &= \tau_{xy}^{(1)} = \mu(u_y + v_z) \\
\tau_{yz}^{(1)} &= \tau_{zy}^{(1)} = \mu(v_z + w_x) \\
\tau_{zx}^{(1)} &= \tau_{xz}^{(1)} = \mu(w_x + u_z)
\end{align*}
\] (4.33)

and

\[
\begin{align*}
n_x^{(1)} &= kT_x \\
n_y^{(1)} &= kT_y \\
n_z^{(1)} &= kT_z
\end{align*}
\] (4.34)

where \(\partial_i = \frac{\partial}{\partial x_i}, \partial_j = \frac{\partial}{\partial y_j}\) and \(\partial_k = \frac{\partial}{\partial z_k}\).

The Second Order Terms of \(\tau^{(2)}_{ij}\) and \(n_j^{(2)}\)

The general expressions for \(\tau^{(2)}_{ij}\) and \(n_j^{(2)}\) in the Burnett equations were first
derived by Burnett in 1935 and later completed by Chapman (Chapman and Cowling 1970) in 1939 and corrected by Wang Chang (Wang Chang and Uhlenbeck 1970) in 1948. They are the conventional Burnett equations written as

\[
\tau_{ij}^{(3)} = -\frac{\mu^2}{p} \left[ \omega_1 \frac{\partial u_j}{\partial x_a} \left( D_{ij} - \frac{1}{3} D_{aa} \delta_{ij} \right) + \omega_2 \left( L_{ij} - \frac{1}{3} L_{aa} \delta_{ij} \right) - \omega_3 \left( M_{ij} - \frac{1}{3} M_{aa} \delta_{ij} \right) \right] \\
-2\omega_1 \left( N_{ij} - \frac{1}{3} N_{aa} \delta_{ij} \right) + \omega_4 R \left( A_{ij} - \frac{1}{3} A_{aa} \delta_{ij} \right) + \omega_5 \frac{1}{\rho T} \left( B_{ij} - \frac{1}{3} B_{aa} \delta_{ij} \right) \\
+ \omega_6 R \left( C_{ij} - \frac{1}{3} C_{aa} \delta_{ij} \right) + \omega_7 \left( E_{ij} - \frac{1}{3} E_{aa} \delta_{ij} \right) \\
(4.35)
\]

\[
q_{ij}^{(2)} = -\frac{\mu^2}{\rho} \left[ \theta_1 \frac{1}{T} \frac{\partial T}{\partial x_i} \frac{\partial u_{ia}}{\partial x_j} + \theta_2 \frac{1}{T} \frac{2}{3} \frac{\partial}{\partial x_j} \left( T \frac{\partial u_{ia}}{\partial x_j} \right) \right] \\
+ \theta_3 \frac{1}{\rho} \frac{\partial p}{\partial x_a} \left( D_{ij} - \frac{1}{3} D_{aa} \delta_{ij} \right) + \theta_4 \frac{\partial}{\partial x_j} \left( D_{ij} - \frac{1}{3} D_{aa} \delta_{ij} \right) \\
+ \theta_5 \frac{1}{T} \frac{\partial T}{\partial x_i} \left( D_{ij} - \frac{1}{3} D_{aa} \delta_{ij} \right) \\
(4.36)
\]

where

\[
L_{ij} = \frac{1}{2} \frac{\partial}{\partial x_i} \left( -\frac{1}{\rho} \frac{\partial p}{\partial x_j} \right) + \frac{1}{2} \frac{\partial}{\partial x_j} \left( -\frac{1}{\rho} \frac{\partial p}{\partial x_i} \right) \\
(4.37)
\]

\[
M_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_a} \frac{\partial u_j}{\partial x_j} + \frac{\partial u_j}{\partial x_a} \frac{\partial u_i}{\partial x_i} \right) \\
(4.38)
\]

\[
N_{ij} = \frac{1}{2} \left[ \frac{\partial u_i}{\partial x_j} \left( D_{ij} - \frac{1}{3} D_{aa} \delta_{ij} \right) + \frac{\partial u_j}{\partial x_i} \left( D_{ij} - \frac{1}{3} D_{aa} \delta_{ij} \right) \right] \\
(4.39)
\]

\[
A_{ij} = \frac{\partial^2 T}{\partial x_i \partial x_j} \\
(4.40)
\]

\[
B_{ij} = \frac{1}{2} \left( \frac{\partial p}{\partial x_i} \frac{\partial T}{\partial x_j} + \frac{\partial p}{\partial x_j} \frac{\partial T}{\partial x_i} \right) \\
(4.41)
\]

\[
C_{ij} = \frac{\partial T}{\partial x_i} \frac{\partial T}{\partial x_j} \\
(4.42)
\]
and $D_q$ is as defined in equation (4.32). The coefficients, $\omega's$ and $\vartheta's$, are gas model constants. They can be calculated by the Chapman-Enskog expansion with a molecular repulsive force model. In the book of *The Mathematical Theory of Nonuniform Gases* (Chapman and Cowling 1970), the coefficients for two theoretical gas models, HS model and Maxwellian model, are obtained. The parameters for the Maxwellian gas are given in Table 4. Since the molecular model for a real gas falls in between these two theoretical models, Lumpkin (1990) obtained the approximate values of $\omega's$ and $\vartheta's$ for the real gas by interpolating linearly in the temperature-viscosity exponent $\omega$ between the two theoretical models. In three-dimensional Cartesian coordinates, the second order constitutive relations can be expressed as

$$E_q = (D_{ia} - \frac{1}{3} D_{a\lambda} \delta_{ia}^\lambda) (D_{a\nu} - \frac{1}{3} D_{\nu\kappa} \delta_{a\nu}^\kappa)$$  \hspace{1cm} (4.43)
\[ \tau_{xx}^{(2)} = -\frac{\mu^2}{p} [a_1u_x^2 + a_2(u_x^2 - w_x^2) + a_3(v_x^2 + w_x^2) + a_4(v_x^2 + w_x^2) + a_6(u_y^2 + v_y^2) + a_7(u_y^2 + v_y^2) + a_8w_yw_z + a_9(v_x + w_x) + a_10RT_x + a_{11}R(T_y + T_z) + a_{12} \frac{RT}{\rho} \rho_x] + a_{13} \frac{RT}{\rho} (\rho_x + \rho_y) + a_{14} \frac{RT}{\rho^2} \rho_z^2 + a_{15} \frac{RT}{\rho^2} (\rho_y^2 + \rho_z^2) + a_{16} \frac{R}{\rho} T_x \rho_x + a_{17} \frac{R}{\rho} (T_y \rho_y + T_z \rho_z) + a_{18} \frac{R}{T} T_x^2 + a_{19} \frac{R}{T} (T_y^2 + T_z^2) \] (4.44)

\[ \tau_{yy}^{(2)} = -\frac{\mu^2}{p} [a_1v_y^2 + a_2(v_y^2 + v_z^2) + a_3(u_y^2 + w_y^2) + a_4(u_y^2 + w_y^2) + a_6(u_x^2 + w_z^2) + a_7(u_x^2 + w_z^2) + a_8u_xw_z + a_9(u_x + w_x) + a_{10}RT_y + a_{11}R(T_x + T_z) + a_{12} \frac{RT}{\rho} \rho_y] + a_{13} \frac{RT}{\rho} (\rho_x + \rho_y) + a_{14} \frac{RT}{\rho^2} \rho_z^2 + a_{15} \frac{RT}{\rho^2} (\rho_x^2 + \rho_z^2) + a_{16} \frac{R}{\rho} T_y \rho_y + a_{17} \frac{R}{\rho} (T_x \rho_x + T_z \rho_z) + a_{18} \frac{R}{T} T_y^2 + a_{19} \frac{R}{T} (T_x^2 + T_z^2) \] (4.45)

\[ \tau_{zz}^{(2)} = -\frac{\mu^2}{p} [a_1w_z^2 + a_2(w_z^2 + w_y^2) + a_3(u_z^2 + v_z^2) + a_4(u_z^2 + v_z^2) + a_6(u_x^2 + v_x^2) + a_7(u_x^2 + v_x^2) + a_8u_xv_x + a_9u_xv_x + a_{10}RT_z + a_{11}R(T_x + T_y) + a_{12} \frac{RT}{\rho} \rho_z] + a_{13} \frac{RT}{\rho} (\rho_x + \rho_y) + a_{14} \frac{RT}{\rho^2} \rho_y^2 + a_{15} \frac{RT}{\rho^2} (\rho_x^2 + \rho_y^2) + a_{16} \frac{R}{\rho} T_z \rho_z + a_{17} \frac{R}{\rho} (T_x \rho_x + T_y \rho_y) + a_{18} \frac{R}{T} T_z^2 + a_{19} \frac{R}{T} (T_x^2 + T_y^2) \] (4.46)

\[ \tau_{xy}^{(2)} = \tau_{yx}^{(2)} = -\frac{\mu^2}{p} [b_1(u_xu_y + v_xv_y) + b_2(w_xw_y + v_xw_y + u_xw_y) + b_3(u_xv_x + u_yv_y) + b_4(u_xv_x + u_yv_y) + b_5(u_xv_x + u_yv_y) + b_6RT_{xy} + b_7 \frac{RT}{\rho} \rho_y] + b_8 \frac{R}{T} T_xT_y + b_9 \frac{RT}{\rho^2} \rho_x \rho_y + b_{10} \frac{R}{\rho} (\rho_x \rho_y + \rho_y \rho_z) \] (4.47)
\[ \tau_{xx}^{(2)} = \tau_{xx}^{(2)} \]
\[ = -\frac{\mu^2}{\rho} \left[ b_1 (u_x u_x + w_x w_x) + b_2 (v_x v_x + v_y v_y) + b_3 (u_x w_x + u_y w_y) \right. \]
\[ + b_4 u_x w_y + b_4 (v_y w_y + u_x v_x) + b_5 R T_{xx} + b_7 \left. \right] + b_7 \frac{R T}{\rho} \rho_{xx} \]
\[ + b_8 \frac{R T}{\rho^2} \rho_x \rho_x + b_9 \frac{R T}{\rho^2} \rho_x \rho_x \]
\[ + b_{10} \frac{R}{\rho} (\rho_x \rho_x + \rho_x \rho_x) \]
\[ (4.48) \]
\[ \tau_{xy}^{(2)} = \tau_{xy}^{(2)} \]
\[ = -\frac{\mu^2}{\rho} \left[ b_1 (v_y v_x + w_y w_x) + b_2 (u_x u_x + u_y v_x + u_y w_y) + b_3 (v_y v_x + v_z v_z) \right. \]
\[ + b_4 v_y w_x + b_3 (u_y v_x + u_x w_x) + b_5 R T_{xy} + b_7 \left. \right] + b_7 \frac{R T}{\rho} \rho_{xy} \]
\[ + b_8 \frac{R T}{\rho^2} \rho_x \rho_y + b_9 \frac{R T}{\rho^2} \rho_x \rho_y \]
\[ + b_{10} \frac{R}{\rho} (\rho_x \rho_y + \rho_x \rho_y) \]
\[ (4.49) \]
\[ q_x^{(2)} = -\frac{\mu^2}{\rho} \left[ c_1 u_x + c_2 (u_y + u_z) + c_3 (v_y + w_x) + c_4 \frac{1}{T} u_x T_x \right. \]
\[ + c_5 \frac{1}{T} (v_y T_x + w_x T_x) + c_6 \frac{1}{T} (u_x T_y + u_x T_y) \]
\[ + c_7 \frac{1}{T} (v_x v_y + w_x w_y) + c_8 \frac{1}{\rho} (v_y \rho_x + u_y \rho_y) + c_9 \frac{1}{\rho} (v_x \rho_x + w_x \rho_x) \]
\[ + c_{10} \frac{1}{\rho} [(u_y \rho_x + u_x \rho_y) + (v_x \rho_x + w_x \rho_x)] \]
\[ (4.50) \]
\[ q_y^{(2)} = -\frac{\mu^2}{\rho} \left[ c_1 v_y + c_2 (v_x + v_z) + c_3 (u_x + w_y) + c_4 \frac{1}{T} v_y T_y \right. \]
\[ + c_5 \frac{1}{T} (u_y T_y + w_y T_y) + c_6 \frac{1}{T} (v_y T_x + v_x T_x) \]
\[ + c_7 \frac{1}{T} (u_x v_y + w_x v_y) + c_8 \frac{1}{\rho} (v_y \rho_x + u_y \rho_y) + c_9 \frac{1}{\rho} (u_x \rho_x + w_x \rho_x) \]
\[ + c_{10} \frac{1}{\rho} [(v_x \rho_x + v_y \rho_y) + (u_x \rho_x + w_y \rho_y)] \]
\[ (4.51) \]
where the coefficients $a's$, $b's$ and $c's$ are given as,

\[
\begin{align*}
    a_1 &= \frac{2}{3} \omega_1 - \frac{14}{9} \omega_2 + \frac{2}{9} \omega_6 \\
    a_2 &= \frac{1}{3} \omega_2 + \frac{1}{12} \omega_6 \\
    a_3 &= -\frac{2}{3} \omega_2 + \frac{1}{12} \omega_6 \\
    a_4 &= -\frac{1}{3} \omega_1 + \frac{7}{9} \omega_2 - \frac{1}{9} \omega_6 \\
    a_5 &= \frac{1}{3} \omega_2 - \frac{1}{6} \omega_6 \\
    a_6 &= \frac{1}{3} \omega_1 + \frac{2}{9} \omega_2 - \frac{2}{9} \omega_6 \\
    a_7 &= -\frac{2}{3} \omega_2 + \frac{1}{6} \omega_6 \\
    a_8 &= -\frac{2}{3} \omega_1 - \frac{4}{9} \omega_2 + \frac{4}{9} \omega_6 \\
    a_9 &= \frac{4}{3} \omega_2 - \frac{1}{3} \omega_6 \\
    a_{10} &= -\frac{2}{3} \omega_2 + \frac{2}{3} \omega_3 \\
    a_{11} &= \frac{1}{3} \omega_2 - \frac{1}{3} \omega_3 \\
    a_{12} &= -\frac{2}{3} \omega_2 \\
    a_{13} &= \frac{1}{3} \omega_2 \\
    a_{14} &= \frac{2}{3} \omega_2 \\
    a_{15} &= -\frac{1}{3} \omega_2 \\
    a_{16} &= -\frac{2}{3} \omega_2 + \frac{2}{3} \omega_4 \\
    a_{17} &= \frac{1}{3} \omega_2 - \frac{1}{3} \omega_4 \\
    a_{18} &= \frac{2}{3} \omega_4 + \frac{2}{3} \omega_5 \\
    a_{19} &= -\frac{1}{3} \omega_4 - \frac{1}{3} \omega_2 \\
    a_{20} &= \frac{2}{3} \omega_4 + \frac{2}{3} \omega_5 \\
\end{align*}
\]
The Augmented Burnett Terms of $r^{(a)}$ and $q^{(a)}$

Equations (4.24-26) with terms of the second-order viscous stress $r^{(b)}$ and the second-order heat flux $q^{(b)}$ are the conventional Burnett equations, where

\[
\begin{align*}
    b_1 &= \frac{1}{2} \omega_1 - \frac{5}{3} \omega_2 + \frac{1}{6} \omega_6 \\
    c_1 &= \frac{2}{3} \varrho_2 + \frac{2}{3} \varrho_4 \\
    b_2 &= -\omega_2 + \frac{1}{4} \omega_6 \\
    c_2 &= \frac{1}{2} \varrho_4 \\
    b_3 &= \frac{1}{2} \omega_1 - \frac{2}{3} \omega_2 + \frac{1}{6} \omega_6 \\
    c_3 &= \frac{2}{3} \varrho_3 + \frac{1}{6} \varrho_4 \\
    b_4 &= \frac{1}{4} \omega_6 \\
    c_4 &= \varrho_1 + \frac{2}{3} \varrho_2 + \frac{2}{3} \varrho_3 + \frac{2}{3} \varrho_5 \\
    b_5 &= \frac{1}{2} \omega_1 + \frac{1}{3} \omega_2 - \frac{1}{3} \omega_6 \\
    c_5 &= \varrho_1 + \frac{2}{3} \varrho_2 - \frac{1}{3} \varrho_3 - \frac{1}{3} \varrho_5 \\
    b_6 &= -\omega_2 + \omega_3 \\
    c_6 &= \frac{1}{2} \varrho_3 + \frac{1}{2} \varrho_5 \\
    b_7 &= -\omega_2 \\
    c_7 &= 2 \varrho_3 + \frac{1}{2} \varrho_5 + \frac{1}{2} \varrho_5 \\
    b_8 &= \omega_4 + \omega_5 \\
    c_8 &= \frac{2}{3} \varrho_3 \\
    b_9 &= \omega_2 \\
    c_9 &= -\frac{1}{3} \varrho_3 \\
    b_{10} &= -\frac{1}{2} \omega_2 + \frac{1}{2} \omega_4 \\
    c_{10} &= \frac{1}{2} \varrho_3 
\end{align*}
\]

It has been shown by Zhong et al. (1991) that the linearized conventional Burnett
equations are unstable to disturbance of small wavelengths. That is, there are some stability problems when the computational grids are made progressively small to solve the conventional Burnett equations. They subsequently proposed augmented Burnett equations to stabilize the conventional Burnett equations while maintaining the second order accuracy of the Burnett level of approximations. The augmented Burnett equations are formed by augmenting the conventional Burnett viscous stress and heat flux terms with linear third-order terms from the super Burnett equations. But these linear third-order terms have different coefficients from those of super Burnett equations and they are determined by carrying out a linearized stability analysis of the augmented Burnett equations. The resulting constitutive relations, $\tau_{y}^{(A)}$ and $q_{j}^{(A)}$, for the augmented Burnett equations are as follows

\[
\begin{align*}
\tau_{y}^{(A)} &= \tau_{y}^{(B)} + \tau_{y}^{(e)} \\
q_{j}^{(A)} &\approx q_{j}^{(B)} + q_{j}^{(e)}
\end{align*}
\]  

(4.54)

where the $\tau_{y}^{(B)}$ and $q_{j}^{(B)}$ are given in equation (4.53), and the general augmented Burnett terms $\tau_{y}^{(e)}$ and $q_{j}^{(e)}$ are

\[
\begin{align*}
\tau_{y}^{(e)} &= -\frac{\mu^3}{p} \left[ \frac{3}{2} \omega_{y} RT (\mathbf{O}_{y} - \frac{1}{3} \mathbf{O}_{aa} \delta_{y}) \right] \\
q_{j}^{(e)} &= -\frac{\mu^3}{p \rho} [\theta_{e} \frac{RT}{\rho} \frac{\partial}{\partial x_{j}} (\frac{\partial^2 \rho}{\partial x_{a} \partial x_{a}}) + \theta_{l} R \frac{\partial}{\partial x_{j}} (\frac{\partial^2 T}{\partial x_{a} \partial x_{a}})]
\end{align*}
\]  

(4.55) \hspace{1cm} (4.56)

where

\[
\mathbf{O}_{y} = \frac{1}{2} \left[ \frac{\partial}{\partial x_{j}} \left( \frac{\partial^2 u_{y}}{\partial x_{a} \partial x_{a}} \right) + \frac{\partial}{\partial x_{i}} \left( \frac{\partial^2 u_{j}}{\partial x_{a} \partial x_{a}} \right) \right]
\]

(4.57)

Here the coefficients $\omega_{y}$, $\theta_{e}$ and $\theta_{l}$ are chosen to stabilize the conventional Burnett
equations. The most natural choice of these coefficients would be the same as those from the super Burnett equations for Maxwellian gas given as,

$$\omega_r = 2/9, \theta_0 = -5/8 \text{ and } \theta_i = -157/16$$

However, the linearized stability analysis shows that the condition for the augmented Burnett equations with $\omega_r = 2/9$ and $\theta_0 = -5/8$ to be stable is $\theta_i > 5/16$ for one-dimensional (Yun 1999) and two-dimensional (Zhong 1991) problems. Hence the coefficients for the augmented Burnett equations are chosen to be the same as that of Zhong (1991) for a Maxwellian gas; that is,

$$\omega_r = 2/9, \theta_0 = -5/8 \text{ and } \theta_i = 11/16 \quad (4.58)$$

These coefficients have also been proven to be stable for three-dimensional problems (Yun 1999). In three-dimensional Cartesian coordinates, the third order terms in the augmented Burnett equations can be expressed as

$$
\tau^{(s)}_{xx} = \frac{-\mu^3}{p^2} \left[ \omega_r RT u_{xxx} + \omega_r RT (u_{yy} + u_{zz}) - \frac{1}{2} \omega_r RT (v_{yy} + w_{zz}) \right] $$

$$
- \frac{1}{2} \omega_r RT (v_{yy} + v_{zy} + w_{xz} + w_{yz}) \right] $$

$$
\tau^{(s)}_{yy} = \frac{-\mu^3}{p^2} \left[ \omega_r RT v_{yyy} + \omega_r RT (v_{xx} + v_{zz}) - \frac{1}{2} \omega_r RT (u_{xx} + w_{zz}) \right] $$

$$
- \frac{1}{2} \omega_r RT (u_{yy} + u_{xy} + w_{xz} + w_{yz}) \right] $$

$$
\tau^{(s)}_{zz} = \frac{-\mu^3}{p^2} \left[ \omega_r RT w_{zzz} + \omega_r RT (w_{xx} + w_{yy}) - \frac{1}{2} \omega_r RT (u_{xx} + v_{yy}) \right] $$

$$
- \frac{1}{2} \omega_r RT (u_{zz} + u_{yy} + v_{xy} + v_{yz}) \right] $$

(4.59) (4.60) (4.61)
\[ \tau_{xy}^{(a)} = \tau_{yx}^{(a)} = \frac{\mu}{2} \left\{ \frac{3}{4} \omega_x \rho_x + \frac{3}{4} \omega_y \rho_y + \frac{3}{4} \omega_z \rho_z \right\} \]

\[ \tau_{xx}^{(a)} = \tau_{yy}^{(a)} = \frac{\mu}{2} \left\{ \frac{3}{4} \omega_x \rho_x + \frac{3}{4} \omega_y \rho_y + \frac{3}{4} \omega_z \rho_z \right\} \]

\[ \tau_{zz}^{(a)} = \tau_{yy}^{(a)} = \frac{\mu}{2} \left\{ \frac{3}{4} \omega_x \rho_x + \frac{3}{4} \omega_y \rho_y + \frac{3}{4} \omega_z \rho_z \right\} \]

\[ q_x^{(a)} = -\frac{\mu}{2} \left[ \theta_x \frac{RT}{\rho} \rho_{xx} + \theta_y \frac{RT}{\rho} \rho_{yy} + \theta_z \frac{RT}{\rho} \rho_{zz} \right] \]

\[ q_y^{(a)} = -\frac{\mu}{2} \left[ \theta_x \frac{RT}{\rho} \rho_{xx} + \theta_y \frac{RT}{\rho} \rho_{yy} + \theta_z \frac{RT}{\rho} \rho_{zz} \right] \]

\[ q_z^{(a)} = -\frac{\mu}{2} \left[ \theta_x \frac{RT}{\rho} \rho_{xx} + \theta_y \frac{RT}{\rho} \rho_{yy} + \theta_z \frac{RT}{\rho} \rho_{zz} \right] \]

Regarding the super Burnett equations, the one-dimensional expressions for \( \tau_{xy}^{(a)} \) and \( q_x^{(a)} \) were given by Simon (1976) and the general expressions were given by Shavaliev (1978). Also, a Maxwellian molecular model was assumed in both works.

**Slip Flow Boundary Conditions**

Traditionally, the no-VS (velocity slip) condition at a gas-solid interface is enforced in the momentum equation and the analogous no-TJ (temperature jump) condition is applied in the energy equation. The notion underlying the no-VSTJ (velocity slip and temperature jump) condition is that within the fluid there cannot be any finite discontinuities of velocity or temperature. Such discontinuities would...
involve infinite velocity or temperature gradients and produce infinite viscous stress
and heat flux that would destroy the discontinuity in infinitesimal time. The
interaction between a gas particle and a wall is similar to that between neighboring
particles, and therefore no discontinuities are allowed at the gas-solid interface either.
In other words, the fluid temperature must be equal to that of the surface. But strictly
speaking those two boundary conditions are valid only if the fluid flow adjacent to the
surface is in thermodynamic equilibrium, which requires an infinitely high collision
frequency between the gas and the solid surface. In practice, the no-VSTJ condition
leads to fairly accurate predictions as long as $Kn < 0.001$. Beyond that, the collision
frequency is simply not high enough to ensure equilibrium and a certain degree of
tangential-velocity slip and temperature jump must be allowed. This is a case
frequently encountered in MEMS flows.

Assuming isothermal conditions prevail, gas molecules, modeled as rigid
spheres, continuously strike and reflect from a solid surface, just as they continuously
collide with each other. For an idealized perfectly smooth wall, the incident angle
exactly equals the reflected angle and the molecules conserve their tangential
momentum and thus exert no shear on the wall. This is termed specular reflection and
results in complete slip at the wall. For an extremely rough wall, on the other hand,
the molecules reflect at some random angle uncorrelated with their incident angle.
The completely diffuse reflection results in zero tangential momentum for the
reflected fluid molecules to be balanced by a finite slip velocity in order to account
for the shear stress transmitted to the wall. A force balance near the wall leads to the
following expression for the slip velocity

\[ u_s - u_w = \lambda \left( \frac{\partial u}{\partial y} \right)_s \]  

where \( \lambda \) is the mean free path, and \( y \) the wall-normal coordinate. The right-hand side can be considered as the first term in an infinite Taylor series, sufficient if the mean free path is relatively small enough. Equation (4.68) states that significant slip occurs only if the mean velocity of the molecules varies appreciably over a distance of one mean free path. This is the case, for example, in vacuum applications and flow in microdevices. The number of collisions between the fluid molecules and the solid in those cases is not large enough for even an approximate thermodynamic equilibrium to be established. Furthermore, nonlinear terms in the Taylor series would be needed as \( \lambda \) increases and the flow is further away from the equilibrium state.

For real walls some molecules reflect diffusively and some reflect specularly. In other words, a portion of the momentum of the incident molecules is lost to the wall and only a portion is retained in the reflected molecules. The tangential-momentum-accommodation coefficient \( a_v \) is defined as the fraction of molecules reflected diffusively. This coefficient depends on the fluid, the solid and the surface roughness, and has been determined experimentally to be between 0.2 and 0.8 (Arkilic 1997; Arkilic et al. 1997), the lower limit being for exceptionally smooth surfaces while the upper limit is typical of most practical surfaces. The final expression derived by Maxwell for an isothermal wall is

\[ u_s - u_w = \frac{2 - a_v}{a_v} \lambda \left( \frac{\partial u}{\partial y} \right)_s \]  

(4.69)
For $\alpha = 1$, equation (4.69) reverts to (4.68). Similar is the argument for the temperature-jump boundary condition. For real walls, the thermal-accommodation coefficient $a_T$ also depends on the fluid, the solid and the surface roughness, and usually is used as a constant of input data.

Based on the physical analysis above, the slip-wall boundary condition is also a big issue for the microflow simulation in the continuum-transition regime, considering the nonequilibrium effects present for the gas-surface interactions. The no-VSTJ boundary conditions are employed at the wall when solving the Navier-Stokes equations for $Kn < 0.001$. In the continuum-transition regime, these conditions are no longer valid and the boundary conditions on the wall are the VSTJ conditions plus zero normal velocity condition. The VSTJ conditions can be derived by considering a Knudsen layer flow in the surface or by considering momentum and energy balance on the surface (Kennard 1938). Both methods result in similar results for the first-order slip conditions that are generally termed the Maxwell/Smoluchowski slip condition (Kennard 1938, Schaaf and Chambre 1961),

\[
\begin{align*}
    u_g - u_w &= \frac{2-a_s}{a_s} \lambda \left( \frac{\partial u}{\partial y} \right)_w + \frac{3}{4} \frac{\mu}{\rho T} \left( \frac{\partial T}{\partial x} \right)_w, \\
    T_g - T_w &= \frac{2-a_T}{a_T} \frac{2}{\gamma+1} \frac{\lambda}{Pr} \left( \frac{\partial T}{\partial y} \right)_w.
\end{align*}
\]  

(4.70) \hspace{1cm} (4.71)

The subscript $g$ denotes the gas variables adjacent to the wall and $w$ the corresponding values of the wall. $Pr$ is the Prandtl number and $\lambda$ is the mean free path of molecules given by
The second term in the right hand side of equation (4.70) is the *thermal creep*, which generates slip velocity in the fluid opposite to the direction of the tangential heat flux, i.e., flow in the direction of increasing temperature. In MEMS devices, thermal creep is the basis for the so-called Knudsen pump, a device with no moving parts, in which rarefied gas is hauled from one cold chamber to a hot one. Equations (4.70) and (4.71) have been used extensively in computing slip flows by using the Navier-Stokes equations.

The Chapman-Enskog expansion, which leads to the Navier-Stokes equations and the Burnett equations, results in increasingly higher order sets of partial differential equations as the order of approximation becomes higher. As a result, the Burnett equations are a one order higher set of equations than the Navier-Stokes equations. In principle, the Burnett equations require second-order slip conditions derived by solving the Boltzmann equation in the Knudsen layer.

For the higher order Burnett equations, it is expected that additional boundary conditions are necessary in order to obtain a unique set of solutions. However there is no physical basis on how to specify the additional boundary conditions. Currently there is no satisfactory method for formulating these additional boundary conditions for the Burnett equations. Beskok (1996) and Beskok and Karniadakis (1994; 1999) proposed a second-order slip condition for the tangential velocity, which is the second-order extension of the Maxwell/Smoluchowski slip condition as

\[
\lambda = \frac{16\mu}{5\rho \sqrt{2\pi RT}}
\]  

(4.72)
where the superscript * denotes dimensionless quantity, \( \text{Re} \) the Reynolds number, and \( \text{Ec} \) the Eckert number. The parameter \( b \) is a high-order slip coefficient determined from the presumably known no-slip solution. If it is chosen as \( b = u'_w / u'_w \), where the primes denote derivatives with respect to \( y \), equation (4.73) becomes second-order accurate in \( Kn \). But there has not been the corresponding part for the second-order temperature jump condition.

\[
\begin{align*}
  u'_w - u'_w &= 2 - a_v \frac{Kn}{a_v} \left( \frac{\partial u'}{\partial y} \right)_0 + \frac{3}{2\pi} \frac{Kn^2 \text{Re}}{\text{Ec}} \left( \frac{\partial T'}{\partial x} \right)_0 \\
\end{align*}
\]  

(4.73)
CHAPTER V

DSMC SIMULATION OF SUP ERSONIC FLOWS IN MICROCHANNELS

Introduction

Microchannel flows occur in narrow channels with the characteristic length scale varying from 100μm to 0.1 μm. The microchannel is a basic element of microfluidic devices (Guckel et al. 1993). A thorough understanding of the thermal physics of such flows is important in the design, fabrication, and operation of MEMS (Gravesen et al. 1993; Sobek et al. 1994; Ho et al. 1998; Janson et al. 1999).

In most microchannel systems, the mean free path of molecules, $\lambda$, is of the same order of magnitude as the height of the microchannel, $h$. For the fluid flows in such microchannels, the Knudsen number is high and the fluid motions are better described from the molecular point of view, as opposed to from the continuum point of view (Bird 1994). Due to the small physical dimensions of the microchannels, the Reynolds number is rather low (order of 10). The low value of the Reynolds number suggests that the viscous force may dominate over the inertial force and the viscous transport of momentum and heat may become an important aspect of such flows. Maxwell (Garber et al. 1995) studied the near-wall behavior of fluid flow of large $Kn$ and proposed that there might be a finite slip of velocity and a finite jump of temperature for gaseous fluid when the mean free path is large compared to the flow

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dimensions. The large gradients of temperature and velocity may affect the transport of heat and momentum in a manner that is different from those observed in larger systems. As the number of industrial and scientific devices using MEMS increases, a detailed understanding of the fluid dynamics and heat transfer in microchannel flows is becoming increasingly important for an accurate prediction of their performance and for a better design.

In this chapter, the heat transfer characteristics of two-dimensional supersonic flows in microchannel are examined. Particularly, the effects of $Kn$ on the wall heat flux are investigated in detail. The molecular dynamic equations are solved using the DSMC method.

Microchannel Flow Simulations

In the current investigation, we use the DSMC method to simulate the heat transfer and flowfield in two-dimensional supersonic microchannel flows near standard atmospheric conditions. The microchannel geometry with the computational domain and uniform cells is shown in Figure 16. Ahead of the microchannel entrance, there is a free stream with distance equal half of the channel height $h$. The present two-dimensional simulations allow a better use of computer resources for a detailed study of the heat transfer mechanisms in microchannels, which may be significantly different from that in three-dimensional cases (Sobek et al. 1994). In fact, there are many examples of two-dimensional microchannel flows in MEMS. For example, there is the gap flow between rotor and stator in micromotors (Gucket et al. 1993) and microengines (Janson 1999).
The effects of Knudsen number on the flowfield temperature and heat transfer are studied in detail. The value of $Kn$ is changed by varying the channel height, while keeping the channel aspect ratio constant. The shock structure, temperature distribution, and net heat flux on the wall for a range of $Kn$ are examined.

Each computational cell has been divided into two subcells in each direction. In the present simulations, the time step has been chosen such that a typical molecule moves about one fourth of the cell dimension in one computational time step. Nitrogen gas is used and the VHS model (Bird 1994) has been applied in all the simulations.

For the standard atmospheric condition, the number density is high and the mean collision time is in the order of $10^{-10}$ sec. The time step used in the DSMC method, $\Delta t$, should be less than the mean collision time, so that the particle
movement and their collision may be uncoupled, i.e.,

\[ \Delta t_a < \Delta x_a / c_{mp} \]  \hspace{1cm} (5.1)

where \( c_{mp} \) is the most probable speed of molecules. The cell size, \( \Delta x_a \), is taken as less than a half of the mean free path in the current simulations; i.e.,

\[ Kn_c = \lambda / \Delta x_a \geq 2 \]  \hspace{1cm} (5.2)

where \( Kn_c \) is defined as “cell Knudsen number”. Borrowing from the traditional CFD, the constraint of equation (5.1) may be expressed as a Courant-Friedrichs-Lewy (CFL) number. So,

\[ CFL = \frac{c_{mp} \Delta t_a}{\Delta x_a} < 1 \]  \hspace{1cm} (5.3)

Physically, this condition requires the particle to reside in the same cell for at least a few time steps to allow it to interact with other particles. This ensures that its information can be distributed properly throughout the domain of computation. Therefore, for DSMC, the CFL number is not a stability constrain, but rather a physical requirement. Violation of this condition may produce solutions that are not physically realistic. In the simulations that will be presented, the value of CFL is set at about 0.2.

**Boundary Conditions**

The temperature at the upper and the lower walls are set equal. When the simulated particle collides with the wall, the diffuse reflection model is used to determine the reflection. In this model, the emission of the impinging molecules is not
correlated with the pre-impingement state of the molecules. The outgoing velocity is randomly assigned according to a half-range Maxwellian distribution determined by the wall temperature. This is also known as the full thermal and momentum accommodation.

Temperature and Heat Transfer

For equilibrium gases of diatomic molecules, by neglecting the vibrational energy, the temperature can be calculated as,

\[
    T = \frac{(3T_r + \zeta r T_{\text{rot}})}{(3 + \zeta r)}
\]  

(5.4)

where \( T_r \) denotes the translational temperature and \( T_{\text{rot}} \) represents the rotational temperature. They are

\[
\frac{3}{2} k T_r = \bar{m} c^2 \bar{c}_0^2
\]  

(5.5)

\[
T_{\text{rot}} = \frac{2}{k} \left( \bar{e}_{\text{rot}} / \zeta r \right)
\]  

(5.6)

where \( k \) is Boltzmann constant, \( m \) the mass of a molecule, \( c \) the velocity of a molecule, \( c_0 \) the mean velocity of simulated molecules, \( \zeta \), the number of rotational degrees of freedom, and \( e_{\text{rot}} \) rotational energy of an individual molecule. The over bar, \( \bar{()}, \) represents the sample average. For nitrogen, there are two degrees of rotational freedom:

\[
\zeta r = 2
\]  

(5.7)

\[
e_{\text{rot}} = -\ln(R_f) k T
\]  

(5.8)

where \( R_f \) is a single random fraction, and

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The translational energy of an individual molecule

\[ e_v = \frac{3}{2} RT_v \]  

The net heat flux on a wall (1 meter wide) can be evaluated as

\[ q = \frac{[(\sum_{i=0} v_i^{\text{inc}} + \sum_{i=0} v_i^{\text{ref}}) \Delta r] \Delta t(1 - \Delta x) N_0}{\Delta t(1 - \Delta x)} \] 

where \( n \) is the total number of simulated molecules that strike the wall during the sampling, \( N_0 \) is the number of gaseous molecules associated with a computational molecule, and \( \Delta t \) is the time period of the sampling. The subscripts, 'inc' and 'ref', denote the values before and after the impact of molecules on the wall, respectively.

Numerical Results

The flows in microchannels with Knudsen number ranging from 0.031 to 0.186 have been simulated, i.e., Case 1, Case 2, and Case 3. The flow conditions and the channel size are given in Table 5. The aspect ratio of the channels is set at 5 for all cases and rectangular cells (100x60) are used. In the figures presented, the height of the channel, \( h \), has been used for nondimensionalization.

Figure 17 shows the shock structures for the three cases. Case 1 shows that in the immediate upstream region of the leading edges, detached bow shocks are formed due to the viscous boundary layers. For this case with \( Kn=0.031 \), the two bow shocks emitted from the upper and the lower walls intersect near \( x/h=1.35 \). The waves resulting from the intersection of the bow shocks diffuse as they separate and extend.
Table 5
Simulated Cases and Conditions

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>LA (μm)</td>
<td>12</td>
<td>6</td>
<td>2.0</td>
</tr>
<tr>
<td>h (μm)</td>
<td>2.4</td>
<td>1.2</td>
<td>0.4</td>
</tr>
<tr>
<td>Free stream distance (μm)</td>
<td>1.2</td>
<td>0.6</td>
<td>0.2</td>
</tr>
<tr>
<td>Kn</td>
<td>0.031</td>
<td>0.062</td>
<td>0.186</td>
</tr>
<tr>
<td>Total number of particles</td>
<td>12,017</td>
<td>11,854</td>
<td>8,041</td>
</tr>
<tr>
<td>M∞</td>
<td>4.15</td>
<td></td>
<td></td>
</tr>
<tr>
<td>T∞ (K)</td>
<td>300</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tw (K)</td>
<td>323</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Number density (m⁻³)</td>
<td>1.75×10⁻⁵</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mean free path of undisturbed gas (m)</td>
<td>7.4×10⁻⁸</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

toward the wall due to the weakening incident shocks. As the Kn increases, the leading edge shocks thicken and the angle between the shock and the wall increases. As such, the intersection of the bow shocks moves upstream. For Case 3 with Kn=0.186, the intersection cannot be identified due to the large shock thickness. The flow initially decelerates to subsonic speed, followed by acceleration. As will be seen in the following, the deceleration of the flow in the highest Kn case, Case 3, is accompanied by a significant increase in wall heat transfer.

Figure 18 shows the temperature contours. The figure shows the incident bow shocks and the strong temperature gradients across the bow shocks near the leading edges for all cases. As the Kn increases, both the temperature and its gradient increase sharply. It is also apparent that an island of high temperature is formed as the Kn increases and the location of the high temperature island moves upstream as the Kn increases. The formation of the high temperature island is, as was mentioned above,
accompanied by the deceleration of the flow. Also, the thickness of the thermal boundary layers in all the cases can be observed to increase with $Kn$.

Figure 17. Mach number contours.

Figure 18. Temperature contours.
Figure 19 shows the density contours. For $Kn=0.031$ and $Kn=0.062$, the two shocks emanating from the leading edges of the microchannel intersect, and then extend to the wall. This causes the formation of islands of low density near the walls in the first half of the microchannel. Behind the intersection, a region of high density appears. For $Kn=0.186$, the shocks are detached further from the leading edge and they are more diffused. The root of the bow shocks is nearly normal to the channel. The shock layer is much thicker than those for the lower $Kn$ cases. The compression shocks spread over almost a half of the microchannel. As a result, there are no identifiable islands of low density near the wall, as was found in cases with lower $Kn$.

![Figure 19. Density contours.](image)

Figures 20a and 20b show the axial temperature and mean velocity profiles at $x/h=0.5, 1.5, 2.5, 3.5$ and $4.5$. The variation of the temperature profiles, Figure 20a,
Figure 20. Profiles, (a) temperature and (b) velocity.

reveals the development of the thermal region. The case with $Kn=0.031$ shows two local peaks in all the profiles and these peaks tend to merge as the flow develops downstream. A fully developed state has not been reached at the downstream end of the channel. On the other hand, for $Kn=0.062$, the peaks merge at about $x/h=4.5$ and the flow is becoming fully developed. For $Kn=0.186$, the temperature profiles flatten out sooner, and the peak value at the centerline decreases significantly downstream.

Axial velocity profiles are shown in Figure 20b. There is a peak at the centerline for all the cases. The peak values vary little in the downstream direction for the $Kn=0.031$ case. However, the peak values for $Kn=0.186$ are significantly reduced as the flow develops downstream. This may be due to the increase of viscous effects.
with increasing $Kn$. For $Kn=0.186$, both the temperature and the kinetic energy decrease significantly as the flow evolves downstream.

The temperature jump at the wall is shown in Figure 21. $T_g$ denotes the gas temperature at the wall and $T_w$ the constant wall temperature. Figure 21 shows that the temperature jump decreases as the flow develops downstream. The highest temperature jump occurs near the microchannel entrance. As $Kn$ increases, the location of the peak temperature jump moves slightly downstream. Near the outlet of the simulated microchannels, the temperature jumps for the cases with $Kn=0.031$ and $Kn=0.062$ appear reaching an asymptotic value.

![Figure 21. The distribution of temperature jump on the wall.](image)

Figure 22 shows the temperature distribution along the centerline of the microchannels. The multiple plateaus of the centerline temperature for the cases with $Kn=0.031$ and $Kn=0.062$ are related to the intersects of the incident and the reflected
shocks. For $Kn=0.186$, the centerline temperature peaks near $x/h=2.0$ and decreases monotonically thereafter. The value of centerline temperature peak increases with the increasing value of $Kn$. The location of the peak also moves upstream with the increasing $Kn$, agreeing with the observation made earlier that the island of increasingly high temperature moves upstream as the Knudsen number increases.

![Figure 22. The distribution of the centerline temperature.](image)

Figure 22. The distribution of the centerline temperature.

Figure 23 shows the streamwise variation of the heat flux $q$ at the wall. For $Kn=0.031$ and 0.062, the heat flux decreases as the flow develops downstream. For $Kn=0.186$, the streamwise variation is distinctively different from those of the lower $Kn$. After an initial region of small variation, the heat flux increases sharply in the midsection of the microchannel. The heat flux peaks at about $14 \times 10^7$ W/m$^2$. The wall heat transfer then decreases monotonically downstream. The maximum value of the wall heat transfer for $Kn=0.186$ is about 3.5 and 2.3 times those for $Kn=0.031$ and
$Kn=0.062$, respectively, representing a significant increase of heat transfer at high $Kn$.

![Graph showing the distribution of heat flux on the wall.](image)

Figure 23. The distribution of heat flux on the wall.

In order to analyze the heat transfer mechanism on the wall, equation (5.11) is written as

$$
\dot{q} = \frac{nN_0}{\Delta t \cdot (1 \cdot \Delta x)} \left( \Delta \overline{\varepsilon}_u + \Delta \overline{\varepsilon}_{rot} \right)
$$

(5.12)

where,

$$
\Delta \overline{\varepsilon}_u = \left[ \left( \sum_{i=1}^{n} \varepsilon_{u, inc} \right) - \left( \sum_{i=1}^{n} \varepsilon_{u, rot} \right) \right] / n
$$

(5.13)

$$
\Delta \overline{\varepsilon}_{rot} = \left[ \left( \sum_{i=1}^{n} \varepsilon_{rot, inc} \right) - \left( \sum_{i=1}^{n} \varepsilon_{rot, rot} \right) \right] / n
$$

(5.14)

The term, $nN_0 / \Delta t \Delta x$, in equation (5.12) represents the number rate of molecules that impact the wall. $\Delta \overline{\varepsilon}_u$ and $\Delta \overline{\varepsilon}_{rot}$ denote the averaged translational and rotational energy deficit per wall-impacting molecule, respectively.
Figure 24 shows the axial distributions of the averaged translational and rotational energy deficit, $\Delta \bar{E}_t$ and $\Delta \bar{E}_{rot}$, per molecule, normalized by $10^{-20}$. The translational energy deficit increases slightly with the increasing $Kn$ upstream of $x/h=2.0$. On the other hand, the rotational energy deficit does not change in any significant way with $Kn$.

![Figure 24](image)

Figure 24. The averaged translational and rotational energy deficit per molecule that strikes the wall, normalized by $10^{-20}$.

The remaining factor in equation (5.12), the number rate of wall-impacting molecules, $nN_0/\Delta t \Delta x$, nondimensionalized by the free stream number density, $1.75 \times 10^{25}$, is shown in figure 25. For $Kn=0.186$, the distribution is quite different from the other two cases with lower Knudsen numbers. For both $Kn=0.031$ and $0.062$, there is a plateau near $x/H=4.0$. The peak value of the number rate of molecules impacting the wall for $Kn=0.186$ is roughly 1000, and those for $Kn=0.031$ and
$Kn=0.062$ are 400 and 580, respectively. The increase of the number rate of molecules that impact the wall is apparently a dominating factor contributing to the observed increase of wall heat transfer. Recall that there are islands of low density near the walls for the lower $Kn$ cases and these islands of low density were not observed for $Kn=0.186$. It is believed that the high number rate of wall-impacting molecules for the high $Kn$ case (0.186) is related to the general high density in the near wall regions that do not exist in the lower $Kn$ cases.

![Graph](image)

Figure 25. The number rate of molecules that strike the wall normalized by $1.75 \times 10^{25}$.

Concluding Remarks

The results obtained show that the heat transfer characteristics of the microchannel flows can vary significantly with Knudsen numbers. For the two-dimensional supersonic microchannel flows simulated in this study, there is a
significant increase of wall heat transfer with Knudsen number. The results show that the enhanced wall heat transfer is mainly caused by the increased number rate of molecules that impact the wall. As the value of the Knudsen number for a typical MEMS device can be quite high, this unique behavior of the wall heat transfer observed in the present simulations may have a significant bearing on the development and the design of MEMS.
CHAPTER VI

DSMC SIMULATION OF SUBSONIC FLOWS IN MICROCHANNELS

Introduction

The DSMC method (Bird 1976, 1994) has been widely used for problems in, for example, rarefied gas dynamics (Moss et al 1994), contaminant pollution over space platform (Rault and Woronowicz 1995), and aerodynamics of reentry vehicles (Ivanov et al. 1997). Computations of the high-\(Kn\) flow in microchannels have recently been demonstrated (Oh et al. 1995; Piekos and Breuer 1995; Xue et al. 2000; Sun and Faghri 2000). Comprehensive reviews can be found in Muntz (1989) and Oran et al. (1998). DSMC has also been applied successfully in the prediction of the heat transfer of high-speed flows in MEMS (Liou and Fang 2001).

In a DSMC simulation, the numerical treatment of the boundaries of the computational domain is important. At the upstream boundary, the Dirichlet type of boundary conditions has usually been used. At the downstream or exit boundary, one traditional approach is to apply the uniform upstream flow condition at the downstream boundary. In this approach, which is often applied in the simulation of external flows, the downstream boundary is required to be far away from the base region. Another conventional approach is to impose a "vacuum" condition at the downstream boundary, where no molecules are allowed to enter the computational
domain. These treatments of the flow conditions at the boundaries have been applied successfully in high-speed flow calculations (Bird 1994; Moss et al. 1994; Rault and Woronowicz 1995; Oh et al. 1995; Ivanov et al. 1997; Liou and Fang 2001). For low-speed flows in atmospheric operating conditions, such as the flows in MEMS, these boundary conditions become inappropriate.

In a subsonic flow, the flow speed can be much lower than the most probable thermal speed. The boundary treatments mentioned above become physically unrealistic as they do not properly model the mass flux due to thermal fluctuations. It is important to take into account the necessary flow characteristic information at the boundaries of the computational domain for a subsonic flow. Although these issues are well known, methods to impose effectively boundary conditions for DSMC of low speed flows have not been as widely studied as those for continuum CFD. Piekos and Breuer (1995) introduced particles based on the differences between a targeted number density and the values calculated by the ideal gas relations. Nance et al. (1998) applied characteristics-based boundary conditions.

In this study, a new implicit treatment for the upstream and the downstream boundary conditions is proposed for the DSMC of low-speed micro-flows (Liou and Fang 2000; Fang and Liou 2002). Gas molecules are allowed to enter the flow domain from both the upstream inlet and the downstream exit boundaries. The local mean velocities, temperature, and number densities near the subsonic boundaries are used to determine the number of molecules entering the computational domain and their corresponding velocities and internal energies at every sample average step. The
proposed boundary conditions have been validated against micro-Poiseuille flows and micro-Couette flows. With $Kn$ ranging from between 0.06 and 0.72, the heat transfer and flow characteristics of the flows are simulated, and also compared with continuum-based analytical solutions using the Maxwellian first-order and Beskok’s (Beskok et al. 1996) second-order slip boundary conditions. The effects of the Knudsen number and wall temperature on the velocity and temperature variations are examined.

New Implicit Boundary Treatment

Microflows often operate with a given pressure (gradient) at the inlet and the outlet boundaries. The inlet velocity distributions are often not available due to experimental difficulties. In this section, the new implicit treatment for the low-speed inlet and exit boundaries for the DSMC of micro-flows in such operation conditions is described (Liou and Fang 2000; Fang and Liou 2002).

Implicit Velocity Distributions for Entering Molecules

From the microscopic point of view, gas molecules translate, in addition to a mean molecular velocity, by the thermal or random velocity. For flows at high speeds, such as hypersonic flows, the thermal velocity can be smaller in magnitude compared with the mean velocity. For a DSMC simulation of high-speed flow, a conventional approach is to impose a “vacuum” condition at the exit boundary, where no molecules enter the computational domain from the region external to the flow domain. For the low-speed flows in fluidic MEMS, the thermal motion can be of the same order of
magnitude as the mean molecular motion. It then becomes inappropriate to neglect the
mass influxes at a flow boundary.

For an equilibrium gas with a one-dimensional mean flow, the quantities
associated with the molecules entering the computational domain from either the
upstream inlet boundary or the downstream exit boundary can be determined
according to the Maxwellian equilibrium distribution function,

\[ f_0 = \frac{\beta^3}{\pi^{3/2}} \exp(-\beta^2 c'^2) \] (6.1)

where

\[ \beta = 1/\sqrt{2RT} \] (6.2)

\( R \) denotes the universal gas constant, \( c' \) the thermal speed of molecule, and \( T \) gas
temperature. Using the Maxwellian distribution function \( f_0 \), the number flux of the
molecules entering the computational domain can be calculated based on the local
temperature and the mean flow velocity. At either the upstream or the downstream
boundaries, the number flux, \( F_j \), from a boundary cell \( j \) can be written as

\[ F_j = \frac{n_j}{2\sqrt{\pi} \beta_j} \left[ \exp(-s_j^2 \cos^2 \theta) + \sqrt{\pi} s_j \cos \theta [1 + \text{erf}(s_j \cos \theta)] \right] \] (6.3)

where

\[ s_j = U_j \beta_j \] (6.4)

\[ \beta_j = 1/\sqrt{2RT_j} \] (6.5)

"erf" represents the error function, \( n_j \) the number density of molecules in cell \( j \), \( T_j \)
and \( U_j \) denote the local temperature and the streamwise mean velocity component,
respectively. \( s_j \) denotes the molecular speed ratio and \( \beta_j \) is related to the thermal scattering. The value of \( \beta \) is zero for the upstream boundary and \( \pi \) for the downstream exit boundary. The velocity components of the entering molecule can be determined by using the acceptance-rejection method (Bird 1994) and the Maxwellian distribution function.

At the upstream inlet boundary, the streamwise thermal velocity, \( c'_u \), of the molecules entering the computational domain should be found in the interval \([-U_j, \infty)\), with a distribution function,

\[
f_{c'_u} \propto (\beta k'_u + s_j) \exp(-\beta^2 c'_u^2)
\]  

To numerically implement the acceptance-rejection method using equation (6.6), the upper limit of \( \infty \) is replaced by a cutoff value of \( 3c_{mp,j} \), where \( c_{mp,j} \) represents the local most probable thermal speed, or,

\[
c_{mp,j} = \sqrt{2RT_j}
\]  

In other words, the thermal velocity, \( c'_u \), is randomly sampled in the interval \([-U_{in,j}, 3c_{mp,j}]\). The resulting streamwise total velocity, \( c_u = U_{in,j} + c'_u \), of the molecules entering the computational domain becomes:

\[
c_u = (U_{in,j} + 3c_{mp,j})R_f
\]  

\( R_f \) represents a random fraction number. The two cross-stream velocity components are assumed to be of the following form,

\[
c_v = A \cos \varphi
\]

\[
c_w = A \sin \varphi
\]
The magnitude, $A$, lies between 0 and $\infty$, with a distribution function,

$$f_A = \exp(-\beta^2 A^2)$$  \hfill (6.11)

Using the acceptance-rejection method, the magnitude, $A$, can be written as

$$A = \sqrt{-\ln(R_f) / \beta} = \sqrt{-\ln(R_f) c_{mp,j}}$$  \hfill (6.12)

The angle, $\varphi$, is uniformly distributed between 0 and $2\pi$. That is,

$$\varphi = 2\pi R_f$$  \hfill (6.13)

Similarly, at a downstream exit boundary, the streamwise thermal velocity of the molecule entering the computational domain from downstream is set in the interval $[-3c_{mp,j}, -U_{e,j}]$. The resulting distributions of the velocity components for the molecule entering the computational domain become:

$$c_x = (U_{e,j} - 3c_{mp,j}) R_f$$  \hfill (6.14)

$$c_y = A \cos \varphi + V_{e,j}$$  \hfill (6.15)

$$c_z = A \sin \varphi$$  \hfill (6.16)

where, $V_{e,j}$ denotes the computed local mean transverse velocity.

With the vibrational energy neglected, the internal energy of the entering equilibrium gases of diatomic molecule consists of translational energy, $e_t$, and rotational energy $e_{rot}$,

$$e_t = mc^2 / 2$$  \hfill (6.17)

$$e_{rot} = -\ln(R_f) kT_j$$  \hfill (6.18)

where $c$ is the speed of an entering molecule, $m$ the mass of the simulated gas, and $k$ the Boltzmann constant.
In order to implement equations (6.1-18), the number density, temperature, and mean velocity at the flow boundaries are needed. And equation (6.3) can be used to obtain the net mass flux at a subsonic boundary. In the following, the methodologies to determine these mean quantities at the boundaries are described.

**Downstream Pressure Conditions**

As was mentioned previously, it is often the pressure, instead of the velocity, that is given at the downstream exit boundary of microflows. A set of physically reasonable boundary conditions to determine the flow properties with a given pressure is needed. These boundary conditions at the exit are of critical importance to a successful DSMC simulation of microflows.

In continuum CFD, the downstream pressure condition in a subsonic flow can be imposed by using the method of characteristics. Inspired by a characteristic theory (Whitfield and Janus 1984) used in continuum CFD, Nance, et al. (1998) proposed a set of correction equations for the pressure boundary conditions. We begin by applying the correction equations proposed by Nance et al. (1998) for the flow properties at the exit boundary in the following form,

\[
(n_j)^i = n_j^i + \frac{p_j - p_j^k}{m(a_j^i)^2}
\]  

(6.19)

\[
(c_{u,j})^i = c_{u,j}^k + \frac{p_j - p_j}{mn_j^i a_j^k}
\]  

(6.20)

\[
(c_{v,j})^i = c_{v,j}
\]  

(6.21)

\[
(T_j)^i = T_j / [(n_j)^i m R]
\]  

(6.22)
The subscript \( e \) represents quantities at the exit boundary, superscript \( k \) the computed quantities at the \( k \)-th step, and \( a_j^k \) the local exit speed of sound. \( p_e \) denotes the imposed exit pressure. There is little detail given in Nance et al. (1998) regarding the implementation of the equations. The current implementation of the characteristics-based equations (6.19-22) ensures a proper account of the influx of mass from the exit boundary and the overall mass balance in the microchannels. The updated mean quantities are first determined by the following sample average equations

\[
U_j = \frac{1}{N_j} \sum c_s
\]  

\[
V_j = \frac{1}{N_j} \sum c_v
\]  

\[
\rho_j = n_j m
\]  

\[
T_j = (3T_u + \zeta \, T_{rot})/(3 + \zeta_r)
\]  

\[
p_j = n_j k T_j
\]

where \( T_u \) denotes the translational temperature, \( T_{rot} \) the rotational temperature, and \( \zeta_r \) the number of rotational degree of freedom. \( k \) represents the Boltzmann constant. The calculated mean quantities were then used in equations (6.19-22) to determine the number and the velocity distribution of the molecules required to enter the computational domain from the exit boundary. The current treatment of the pressure downstream boundary conditions consists of the following steps:

**Step 1.** Determine the number density of the molecules at the exit by equation (6.19).

A mass conservation is then satisfied in the computational domain.
Step 2. Determine the exit temperature by equation (6.22) and the corrected velocity components of the simulated molecules at the boundary cells using equations (6.20) and (6.21).

Step 3. Determine the exit mean flow velocity by sampling.

\[
U_{e,j} = \frac{1}{N_j} \sum c_{u,e}
\]  
\[V_{e,j} = \frac{1}{N_j} \sum c_{v,e}\]

Step 4. The implicitly determined downstream properties can then be used to calculate the number of the entering molecules from the number flux function, equation (6.3), and their velocity components from the velocity distribution functions, equations (6.14-16).

Upstream Mean Flow Conditions

Several types of treatments have been proposed (Nance et al. 1998; Ikegawa and Kobayashi 1990) for the velocity at a subsonic upstream inlet boundary. In Ikegawa and Kobayashi (1990), the mean flow velocity \(U(t)\) at the boundaries was determined based on the number of molecules flowing in, \(N_{in}^{(t-t')}\), and out, \(N_{out}^{(t-t')}\), from the upstream or the downstream boundaries at previous time,

\[
U(t) = \frac{N_{in}^{(t-t')} - N_{out}^{(t-t')}}{n \delta A}
\]

where the molecule number \(N_{in}\) is

\[
N_{in} = F \delta A
\]
$\delta t$ represents a time step and $A$ the boundary cross-section area. $F$ denotes a number flux determined by averaging equation (6.3) over the whole inlet boundary. In a single time step, both $(n \delta t A)$ and $(N_m - N_{om})$ are small and the scattering of $U(t)$ may become rather large, causing the numerical solution to become unstable. Ikegawa and Kobayashi (1990) reduced the scattering by using the average value of two consecutive time steps.

The inflow mean velocity condition used in Nance et al. (1998) is quite similar to that proposed by Ikegawa and Kobayashi (1990). Instead of using a constant mean flow velocity, the particle conservation was applied on a per-cell basis. The particle fluxes were computed from the Maxwellian distribution. In contrast, Ikegawa and Kobayashi determined the particle fluxes by the actual particle counts across the computational boundaries.

A rather simple implicit type of condition is proposed in this work for the mean flow velocity at the upstream inlet. At the upstream boundary, the pressure $p_m$ and density $\rho_m$ are the given parameters of the flow. The number density $n_m$ and temperature $T_m$ can be then obtained according to the mass and the equation of state; i.e.,

$$ (n_m)_j = \rho_m / m \quad (6.32) $$

$$ (T_m)_j = p_m / \rho_m R \quad (6.33) $$

The transverse mean velocity $V_{m,j}$ is set to zero. A first-order extrapolation is used to determine the streamwise mean velocity, $U_{m,j}$, from that of the value computed for
cell \( j \). That is,

\[
U_{m,j} = U_j
\]

where the right-hand-side term is the cell-average velocity of the upstream boundary cells calculated from equation (6.23). This method is commonly used in continuum CFD and has been successful for a wide range of internal as well as external flows. The particle number fluxes and the velocity components of entering molecules were determined locally from the Maxwellian distribution by equation (6.3) and equations (6.8-10), respectively.

It is shown in the following section that the implicit boundary treatment successfully drives a microchannel flow to a stationary state with matching exit pressure and overall mass balance, which are the fundamental criteria for validating internal flow computation. Because of the statistical scatter of the DSMC method, this technique becomes inappropriate for flows of extremely low speeds. The information preservation (IP) method (Cai et al. 2000; Fan and Shen 2001) has been shown to work well in such conditions. In the following, the results for three types of microchannel flow calculations are presented. The effects of the Knudsen number on the heat transfer characteristics are discussed.

**Microflow Predictions**

The new implicit boundary treatment has been implemented into a DSMC code, which was originally developed by Bird (1994). The modified DSMC code has been applied to calculate two types of microflows, the micro-Couette flows and the
micro-Poiseuille flows, as shown in Figure 26. Some of the computational results are presented and, where appropriate, compared with analytical results based on the Navier-Stokes equations with velocity-slip and temperature-jump boundary conditions.

For fully developed parallel flows with low Reynolds numbers, the Navier-Stokes equations can be simplified,

\[
\frac{dp}{dx} = \mu \frac{d^2 u}{dy^2}
\]  \hspace{1cm} (6.35)

For the micro-Couette flow, the pressure gradient is zero and the upper plate moves at a speed of \( U \). Excluding the thermal creep term of equation (4.70), the first-order slip boundary condition of Maxwell/Smoluchowski can be written as

\[
u_s' - u_s' = \frac{2 - a_s}{a_s} Kn \left( \frac{\partial u_s'}{\partial y} \right) x
\]  \hspace{1cm} (6.36)

where the velocity is normalized by \( U \) and \( y \) by the microchannel height \( h \), and the Knudsen number is defined as \( Kn = \lambda / h \). Beskok (1996) proposed a second-order slip boundary condition as,
A distribution of the mean flow velocity, \( u \), for the micro-Couette flow can be obtained by solving equations (6.36) and (6.37), which gives,

\[
\frac{u}{U} = \frac{1}{2 \frac{2-a_v}{a_v} Kn+1} \left( \frac{y}{h} + \frac{2-a_v}{a_v} Kn \right)
\]

Equation (6.38) shows that, according to this continuum-based model, the \( Kn \) of the microflow determines the slope of the velocity profile and the slip velocity on the walls. Note that a use of the second-order slip condition would result in the same velocity distribution as equation (6.38) due to the linear nature of the velocity profile (Beskok 1996).

For a pressure-driven micro-Poiseuille flow, the use of the first-order slip boundary condition results in the following distribution for the mean velocity.

\[
\frac{u}{U} = \frac{h^2}{2 \mu} \frac{dp}{dx} \left[ \left( \frac{y}{h} \right)^2 - \frac{y}{h} \frac{2-a_v}{a_v} Kn \right]
\]

By using the second-order slip boundary condition, equation (6.38), one would obtain a more accurate distribution for the velocity,

\[
\frac{u}{U} = \frac{h^2}{2 \mu} \frac{dp}{dx} \left[ \left( \frac{y}{h} \right)^2 - \frac{y}{h} \frac{2-a_v}{a_v} \frac{Kn}{1+Kn} \right]
\]

Both equations (6.39) and (6.40) show that the velocity is a function of Knudsen number, distance to the wall, as well as pressure gradient. For a full diffusely reflecting wall, \( a_v = 1 \), nondimensional forms of equations (6.39) and (6.40) can be
obtained by using the centerline velocity as the velocity scale. The resulting nondimensional forms of the first-order and the second-order accurate velocity profiles are, respectively,

\[ \frac{u}{u_c} = \left[ -\left( \frac{y}{h} \right)^2 + \frac{y}{h} + Kn \right] \left( \frac{1}{4} + Kn \right) \]  

(6.41)

\[ \frac{u}{u_c} = \left[ -\left( \frac{y}{h} \right)^2 + \frac{y}{h} + \frac{Kn}{1 + Kn} \right] \left( \frac{1}{4} + \frac{Kn}{1 + Kn} \right) \]  

(6.42)

In the slip-flow range with Kn less than 0.1, the continuum-based solution approximates well the microflows and is commonly used for comparison with DSMC results.

Numerical Results and Discussions

In this section, micro-Couette flows and micro-Poiseuille flows with various values for the ratio of wall temperature to the inlet flow temperature are simulated. The VHS model (Bird 1994) and diffusive wall boundary condition are used for the collision processes. Some of the computational results are presented and, where appropriate, compared with analytical results described above.

Micro-Couette Flows

For the simulated micro-Couette flow of nitrogen, the upper wall moves with a speed \( U \) of 100 m/s. The simulated parameters are shown in Table 6. The pressure at the inlet and the outlet boundaries are both set at 0.83 atm (\( p_e = p_o = 0.83 \) atm). The temperature of inlet flow, \( T_i \), and the temperature of the upper and the lower walls,
$T_\text{w}$, are all set equal to 300K. The channel length $L$ is 4.0μm. Two cases were simulated with the channel heights, $h$, of 0.4μm and 0.8μm, respectively. The Knudsen numbers, based on the channel height and the inlet condition, are 0.08 and 0.163. The physical parameters are set such that a low-speed microflow is simulated. The computational grid consists of 100×60 uniform rectangular cells for both cases. The number of simulated molecules is about 320,000. Runs of 200,000 time steps and sampling after 2000 time steps of development on SGI-Octane typically take roughly 48 hours of CPU time with a single processor.

<table>
<thead>
<tr>
<th>Case</th>
<th>Size (μm)</th>
<th>$P_\text{in}/P_e$</th>
<th>$T_\text{in}$ (K)</th>
<th>$T_\text{w}$ (K)</th>
<th>$Kn$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4.0×0.8</td>
<td>1.0</td>
<td>300</td>
<td>300</td>
<td>0.08</td>
</tr>
<tr>
<td>2</td>
<td>4.0×0.4</td>
<td>1.0</td>
<td>300</td>
<td>300</td>
<td>0.163</td>
</tr>
</tbody>
</table>

Figures 27a and 27b show the predicted velocity profiles for $Kn=0.08$ and $Kn=0.163$, respectively. The corresponding linear profiles given in equation (6.39) are also shown for comparison. Overall, there is good agreement between the continuum-based solutions and the DSMC results for $Kn=0.08$, which suggests that the current implicit boundary condition is suitable for DSMC. In the center portion of the channel, the DSMC solution agrees well with the continuum-based linear solution. There appears to be a slight difference between the two solutions away from the center portion. For the case with a higher $Kn$ (0.163), a nonlinear profile was obtained by the DSMC. Compared with the linear, continuum-based solution, the DSMC method has predicted a velocity profile with a lower value of slope in the center.
portion of the channel and with slight curvatures approaching the wall. Figure 27c shows the velocity differences between the DSMC results and the continuum-based analytical solutions across the channel for both cases. The nonlinear, wavy behavior of the DSMC solution is evident, especially for the higher $Kn$ case. The effect of $Kn$ on the micro-Couette flow observed in the present DSMC results has not been reported in prior published articles that we are aware of. The difference in the wall slip velocity between the DSMC and the analytical solution is small. For the higher $Kn$ case (0.163), the calculated slip velocity at the lower wall, 11.87 m/s, is roughly 3% lower than that of equation (6.39). It suggests that the difference between the velocity profiles predicted by the present DSMC method and the analytical form based on the continuum assumption is not necessarily due entirely to the low-order of accuracy in the slip-boundary condition.

![Graph showing velocity profiles for micro-Couette flows, $Kn=0.08$.](image)

Figure 27a. Comparison of the velocity profiles for micro-Couette flows, $Kn=0.08$. 

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Figure 27b. Comparison of the velocity profiles for micro-Couette flows, \( Kn = 0.163 \).

Figure 27c. Velocity difference between the present DSMC and the continuum-based analytical solutions for micro-Couette flows.

The distribution of temperature in the wall-normal direction for the case with a lower \( Kn \) (0.08), at the station \( x/L = 2.5 \), is shown in Figure 28. Also included is an
analytical approximation, which is derived from a simplified form of the Navier-Stokes equations using the first-order wall velocity-slip and the first-order wall temperature-jump condition of Maxwell, equations (4.70) and (4.71). The analytical approximation can be written as,

$$T = T_w + \frac{1}{2} \mu U^2 \left[ \frac{1}{K \left( 2 - \frac{a_t}{\alpha} \frac{Kn}{Pr} + 1 \right)} \right]^\frac{1}{2} \left( \frac{y}{h} \right)^\gamma + \frac{\gamma}{h} \frac{2 - a_T}{a_T} \frac{y}{h} \frac{Kn}{Pr} + 1$$

(6.43)

where $\mu$ represents the viscosity, $a_t$ the coefficient of momentum accommodation, $a_T$ the coefficient of heat accommodation, $K$ the conductivity and $Pr$ the Prandtl number. The values used for $\mu$, $\sigma_r$, $\sigma_T$, $K$, and $Pr$ for nitrogen (Weast et al. 1984) are $1.656 \times 10^{-5} \text{kg/(ms)}$, 1.0, 1.0, 0.023 J/(msK), and 0.72, respectively. The analytical form gives a distribution that, in general, agrees well with the present DSMC results. The wall temperature-jump of about 0.3 K is predicted by both methods. The relative

![Graph showing temperature profile for micro-Couette flow.](image)

Figure 28. Comparison of the temperature profile for micro-Couette flow.
scattering error is less than 0.1%. Results at other locations are similar because of the one-dimensional nature of the micro-Couette flow.

Micro-Poiseuille Flows

Two micro-Poiseuille flows were calculated with parameters shown in Table 7. The height of the micro-channel $h$ is 0.4μm, and the length $L$ is 2.0μm for both cases. The inlet flow temperature is 300K and the wall temperature is 323K. The pressure ratios are 2.5 for Case 1 and 4.5 for Case 2. The inlet pressure is 2.5atm for Case 1 and 0.73atm for Case 2. These operating conditions result in the local $Kn$ in the microchannels varies between 0.055 and 0.123 for Case 1 and between 0.19 and 0.72 for Case 2. The aspect ratio of the microchannels simulated is 5, which is significantly lower than those found in experiments (Arkilic et al. 1994; Harley et al. 1995). The computation grid contains $100 \times 60$ uniform rectangular cells. The number of simulated molecules is about 180,000. Runs of 200,000 time steps, with sampling after 2000 time steps of development, on a SGI-Octane typically take nearly 36 hours of CPU time with a single processor. Significant speedup can be obtained with a parallel version of the DSMC code (Fang and Liou 2002). A multi-fold speedup is normally obtained. The results shown in the following for Case 2 are obtained using a dual-processor SGI-Octane. A constant velocity of 100m/s is used uniformly in the computational region, including the flow boundaries, to initiate the simulation.

Figure 29 shows the evolution of the calculated pressure at the downstream boundary, nondimensionalized by the imposed exit pressure, $p_e$, as the solution
progresses for Case 2. In each print cycle, there are ten time steps of sampling. The calculated pressure converges to the imposed value \( \frac{p}{p_c} \approx 1 \) after a transient variation from the uniform initial conditions has subsided.

Table 7

<table>
<thead>
<tr>
<th>Case</th>
<th>Size (μm)</th>
<th>( P_{in}/P_c )</th>
<th>( T_{in} ) (K)</th>
<th>( T_{w} ) (K)</th>
<th>( Kn )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>2.0 × 0.4</td>
<td>2.5</td>
<td>300</td>
<td>323</td>
<td>0.055–0.123</td>
</tr>
<tr>
<td>Case 2</td>
<td>2.0 × 0.4</td>
<td>4.5</td>
<td>300</td>
<td>323</td>
<td>0.19–0.72</td>
</tr>
</tbody>
</table>

Figure 29. Evolution of the downstream pressure, Case 2.

Figure 30 shows the approach to a steady state solution using the same print cycles as in Figure 29 for Case 2. As was described earlier, an initial velocity field \( U_{\text{initial}} \) is required to start the calculations and \( U_{\text{initial}} = 100 \text{m/s} \) is used. For a pressure-
driven internal flow, this computational initial condition set at the interior flow
domain and the flow boundaries where the boundary treatment is used should have no
bearing on the final numerical solution. For validation, Figures 30 also includes
results for a second $U_{\text{initial}} (=15\text{m/s})$. Figure 30a shows the variation of the mass fluxes
at the upstream and downstream boundaries. The mass flux is defined as,

\[ m = \frac{1}{h} \int_0^L \rho u \, dy \]  \hspace{1cm} (6.44)

The corresponding initial values are denoted by the solid symbols in Figures
30a and 30b. The initial mass flux is about 12kg/ms for the case with $U_{\text{initial}} =15\text{m/s}$
and 80kg/ms for $U_{\text{initial}} =100\text{m/s}$. For both cases Figure 30a shows that, after a
transient from the uniform initial conditions, the mass fluxes at the upstream and the
downstream converge to the same constant value and an overall mass balance in the
microchannel is established. Figure 30a also shows that the converged mass fluxes for
the two different initial fields agree well, which is about 39.4kg/m$^2$s with a 0.25%
variation. Figure 30b shows the variation of the average streamwise velocity for an
inlet cell and an outlet cell located at $(0, h/2)$ and $(L, h/2)$, respectively. For both
initial conditions, the streamwise velocity for the inlet cell converges to 58.78
($\pm0.54\%$) m/s. For the outlet cell, the velocity converges to 232.05 ($\pm0.32\%$) m/s.
These results agree well with Bird’s calculation (Bird 2000) using extended buffer
domains and vacuum boundary conditions. The results shown in Figures 29 and 30
indicate that the present implicit treatment of the low-speed boundaries supports a
stable and efficient solution process for the DSMC of the internal microflows studied.
As is mentioned earlier, boundary conditions previously developed for the DSMC of high-speed flows do not properly model the mass flux due to thermal
fluctuations in flows of low-speed. Figure 31a shows the distribution of the influxes of fluid mass into the computational domain due to the thermal fluctuations, $nmu$, at the upstream and the downstream boundaries for the two micro-Poiseuille flows. The distributions have been normalized by the local mean mass flux. Since the number flux at the boundaries was determined by the local mean properties, the local thermal mass fluxes are not uniformly distributed across the channel. According to the present results, however, the nonuniformity decreases at higher $Kn$. The sectional thermal mass fluxes obtained by integrating the thermal mass flux over the inlet and the outlet boundaries are shown in Figure 31b. At the upstream boundary, the thermal mass flux into the computational domain increases with pressure gradient due to the increased mean velocity. At the downstream boundary, the influx of fluid mass due to thermal fluctuations is nearly 50% of that of the total mass flux for Case 1 and 20% for Case 2. The results show that the thermal mass flux entering the flow domain at a downstream boundary is significant and the "vacuum" boundary condition used for high-speed flows is not physically reasonable to use in the DSMC of the subsonic microchannel flows.

Figure 32a shows the predicted pressure distribution along the channel centerline for Case 1. A continuum-based analytical form (Piekos 1995) obtained using the first-order slip condition was also included for comparison. Figure 32b shows the relative difference of pressure between the DSMC result and the analytical solution. The maximum difference is roughly 2%, indicating that the current boundary treatment is appropriate to use with the DSMC techniques. Both methods predicted
Figure 31a. Local thermal mass flux normalized by mean mass flux for micro-Poiseuille flows.

Figure 31b. Sectional mean thermal mass flux normalized by mean mass flux for micro-Poiseuille flows.
Figure 32a. Comparison of pressure distributions for micro-Poiseuille flow, Case 1.

Figure 32b. Relative difference of pressure between the DSMC result and analytical solution for micro-Poiseuille flow, Case 1.

nonlinear pressure distributions along the channel, which has been observed experimentally in microchannel flows. Figure 32c compares the deviations of the
DSMC and of the analytical pressure drops from the linear distribution, $p_L$. The nonlinearity exhibited by the DSMC is 0.5% lower than that of the continuum-based solution.

![Graph: Comparison of the deviations of DSMC and of the analytical pressure drop from linear distribution for micro-Poiseuille flow, Case 1.](image)

Figure 32c. Comparison of the deviations of DSMC and of the analytical pressure drop from linear distribution for micro-Poiseuille flow, Case 1.

Figure 33 shows a comparison of the DSMC velocity profiles with the continuum-based analytical solution of equations (6.42) and (6.43) at six different locations along the channel. The value of the $Kn$ changes from 0.055 to 0.118. For the small $Kn$, there is little difference between the first- and the second-order accurate continuum-based velocity profiles. The calculated profiles agree well with the continuum solutions for all the stations compared. In this low $Kn$ range, the continuum-based analytical result provides an approximated solution to the microflow considered. Results show that the present implicit treatment of the upstream and the downstream boundary conditions is consistent with the DSMC procedure and has
produced accurate numerical predictions to the microflows considered.

Figure 33. Comparison of velocity profiles of micro-Poiseuille flow, Case 1.
In Case 2 the local $Kn$ is higher than Case 1. Figure 34a shows the pressure
distribution along the centerline of the channel. Figure 34b shows the difference of
pressure distribution between the DSMC solutions and the continuum-based form,
with a maximum difference of 3%. Compared with Case 1, a stronger nonlinearity is
predicted by both methods. Figure 34c shows that the deviation from the linear
distribution is 9% for the DSMC results and 10% for the continuum-based results.

Figure 35 shows the calculated mean velocity profiles at six different stations
along the channel, compared with analytical solutions of the first-order and the
second-order slip-wall conditions. The differences between the first-order profiles and
the second-order profiles for this case are more significant than those for Case 1.
While the second-order profiles give reasonable approximations to the DSMC results
for $Kn$ up to 0.641, the first-order profiles move away from the DSMC results as the
value of the $Kn$ increases, with the highest difference occurring at the channel wall.

![Figure 34a](image-url)  
Figure 34a. Comparison of pressure distributions for micro-Poiseuille flow, Case 2.

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Figure 34b. Relative difference of pressure between the DSMC result and analytical solution for micro-Poiseuille flow, Case 2.

Figure 34c. Comparison of the deviations of DSMC and of the analytical pressure drop from linear distribution for micro-Poiseuille flow, Case 2.
Figure 35. Comparison of velocity profiles of micro-Poiseuille flow, Case 2.
Figure 36 shows the variations of the gas slip-velocity along the wall for both cases. The slip-velocity is defined as,

\[ u_s = u_g - u_w \]  

(6.45)

where \( u_g \) represents the gas velocity adjacent to a wall and \( u_w \) the wall velocity. It can be seen that the slip-velocity increases as the flow develops downstream. For the high Kn case, Case 2, the increase is more significant. At the exit of the microchannel, the slip-velocity for Case 2 is nearly twice as high as that of Case 1.

![Figure 36. Slip velocity on the wall.](image)

Analytical forms of the slip-velocity distribution can be obtained from equations (6.41) and (6.42) by setting \( y = 0 \). The resulting wall slip-velocity can be written as,

\[ \frac{u_s}{u_c} = Kn \left( \frac{1}{4} + Kn \right) \]  

(6.47)

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where $Kn$ is also the local Knudsen number on the wall, which varies with the flow developing downstream. Equation (6.47) is obtained by using the first-order slip-wall condition proposed by Maxwell and equation (6.48) by using a high-order condition.

In Figure 37, the wall slip-velocity given by equations (6.47) and (6.48) are compared with the present DSMC predictions. For Case 1 with the lower $Kn$, the continuum-based analytical values agree well with the DSMC results in the entire microchannel. As the $Kn$ is low, it is not surprising to observe such a good agreement between the continuum-based solutions and the current DSMC results. This agreement also further validates the DSMC solver used in the present study. The difference between the first-order and the high-order approximations becomes more apparent for Case 2, where the $Kn$ is large (>0.19). In fact, Figure 37 shows that the first-order approximation is no longer valid for Case 2, producing a velocity slip significantly higher than both the DSMC result and the high-order analysis.

Figure 38 shows the contours of the streamwise mean velocity magnitude for Case 1 and Case 2. The flow velocity increases as it develops downstream. Partly due to the high-pressure gradient, the flow speed at the exit of Case 2 is higher than that of Case 1. There is only small statistical scatter in the computed velocity for both cases.
First-order analysis
High-order analysis

Figure 37. Comparison of normalized slip velocity distributions.

Figure 38. Streamwise velocity magnitude contours.

The difference between the wall temperature and the gas temperature near the wall, or the temperature-jump, for these two cases are given in Figure 39. For both
cases, there is a gradual decrease of temperature-jump in the first half of the channel, from about 10K to nearly the same, suggesting a corresponding gradual decrease of the heat transfer from the wall to the microflow. In the second half of the channel, the wall temperature-jump for Case 2 shows a significant increase as the flow develops toward the exit than that for Case 1.

![Figure 39. Wall temperature-jump.](image)

The calculated distributions of temperature are shown in Figure 40. The flows are seen to have an increase of temperature as the flow develops in the first half of the channel. This is likely to be caused by the temperature difference between the wall and the flow. The contours, however, show a subsequent decrease of temperature in the downstream half of the microchannel for both cases, with a more pronounced reduction in Case 2. A different view of the temperature distribution is given in Figure 41. The temperature distribution across the channel for these two cases
develops in a similar manner before $x/h=3.0$. Further downstream, the temperature decreases, with a more significant reduction for Case 2 with higher $Kn$. Near the exit, the temperature in the centerline region of Case 2 is about 15K lower than that predicted for Case 1.

Figure 40. Temperature contours.
Figure 41. Comparison of temperature profiles.
Figure 42 shows the wall heat transfer distributions. The net heat flux on a wall element with length $\Delta x$ can be evaluated as,

$$
\dot{q} = \frac{n}{t_s(1 \cdot \Delta x)} \left[ \sum_{i=1}^{n} (e_{r,i} + e_{r,ref})_{inc} - \sum_{i=1}^{n} (e_{r,i} + e_{r,ref})_{ref} \right] \cdot N_0
$$

(6.49)

where $n$ is the total number of simulated molecules that strike the wall element during sampling, $N_0$ the number of gaseous molecules associated with a simulated molecule and $t_s$ the time period of the sampling. The subscripts “inc” and “ref” denote the values before and after the molecule impacts the wall, respectively. Near the entrance region, there is significant transfer of heat from the wall for both cases due to the high wall temperature. The level is higher for Case 1 than for Case 2 with higher $Kn$. As the flow develops downstream the wall heat transfer diminishes and the difference between Case 1 and Case 2 falls within statistical error. The results suggest that the flow expansion observed in Figure 38 in the second half of the channel is nearly adiabatic for both cases, despite the finite temperature-jump at the wall. This is particularly true for Case 2. Recall that the gas temperature near the exit for Case 2 is lower than that for Case 1 by about 15K and lower than the wall temperature by about 40K. This result suggests that, for the high $Kn$ case (Case 2), the large temperature difference between the wall and the flow is not accompanied by any significant amount of wall heat transfer. Note that the heat transfer characteristics of supersonic flows with three different values of $Kn$ in a microchannel have been studied in Chapter 5 (Liou and Fang 2001). For the case with the highest $Kn$ (0.186), the results showed a significant increase of wall heat transfer with large temperature difference.
between the wall and the flow. On the other hand, the temperature along the streamwise direction develops in a manner similar to the current low-speed cases. That is, the temperature for the flow with large $Kn$ is higher than that with low $Kn$ at the upstream and, as the flow develops downstream, a more substantial drop of the flow temperature is found for cases with high $Kn$. These computational results appear to indicate that the heat transfer characteristics of high $Kn$ microfluid flows at low speeds can be different from that at high speeds. A detailed, systematic study is apparently needed to gain a better understanding of the possible differences in the heat transfer characteristics between low-speed and high-speed microchannel flows.

![Figure 42. Wall heat transfer.](image)

**Concluding Remarks**

A new implicit treatment of the boundary conditions for the DSMC of low-
speed MEMS flows has been presented. The local mean velocity, temperature and number density near the boundaries were used to determine the number of molecules entering the computation domain and their corresponding velocities and internal energies. The pressure exit condition has been physically imposed. The method enforces mass conservation and is consistent with the characteristic theory of subsonic flows.

Micro-Couette flows and micro-Poiseuille flows were computed and compared with analytical solutions derived from the Navier-Stokes equations using slip-boundary conditions. The results show that the proposed implicit treatment of subsonic flow boundaries is robust and appropriate for DSMC simulation of the flows in MEMS.

The DSMC results indicate that the velocity profile of the micro-Couette flow exhibits a nonlinear wavy behavior that has not been reported previously. The results also show that the mass influx due to thermal fluctuations represents a significant portion of the overall mass flux balance in subsonic MEMS flows.

The thermal dynamics of the computed flows are also examined. The wall heat transfer in the calculated subsonic microfluid flows decreases with an increase of Knudsen number. The present results show that the Knudsen number has significant effects on the fluid dynamic and the thermodynamic behavior of the microfluid flows studied.
CHAPTER VII

PARALLEL DSMC SIMULATION OF MICROFLOWS

Introduction

The DSMC method (Bird 1994) is one of the most widely used methods for analyzing hypersonic rarefied gas flows (Moss et al. 1994). The method has been applied to a range of problems, for example, contaminant pollution over space platforms (Rault and Woronowicz 1995). Recent advances have resulted in procedures more efficient for dealing with complex three-dimensional geometry as well as significant reductions in the computational effort. Such advances have made practical the applications of DSMC to the calculations of the rarefied gas flow over the full Space Shuttle geometry (Bird 1990).

For microfluid flows in MEMS, the operating pressure is either near or higher than the atmospheric pressure. Using DSMC to calculate such flows of high density can be quite demanding in both the computer memory and the computational time. Methods to deal with large variation in density have been proposed and applied successfully to many problems. These schemes generally require a significant amount of computer time for near-continuum conditions due to, partly, the increase of the collision frequency at high gas density. As such, further reductions in computational time are still in need to make the calculations of high-density, large-scale microfluid
flow problems more affordable.

Parallel implementations of DSMC for high-speed rarefied gas applications have been reported in the literature (Wilmoth and Carlson 1992; Dietrich and Boyd 1995; LeBeau 1999). The computer platforms used include, for example, IBM SP-2 and CRAY-T3E. In recent years, hardware for personal computer (PC) has dramatically improved. This, when coupled with efficient algorithms for parallel implementation, offers a tremendous potential for a significant reduction of computation time for the DSMC of microfluid flows in a cost-effective manner. In fact, massive parallelization can achieve and even surpass the performance of the current supercomputers for certain types of problems.

This chapter presents the basic implementation of a parallel algorithm for DSMC and the results of its applications to microfluid flows. The implementation of the parallel algorithm does not require any major changes to the procedures of DSMC and can, in principle, be applied to the general codes. Such an implementation will allow a wider range of flow conditions to be studied and make possible a direct comparison of the DSMC results with the continuum Navier-Stokes or Burnett equations solutions for microfluid flow problems.

In the following, the algorithm of parallel DSMC (PDSMC) method for microflows is described. Results of performance benchmarking on a Pentium III PC cluster are presented. The performance and the efficiency are examined, which include a straight microchannel and a microchannel with a patterned surface structure. The benchmark results show significant advantages that can be gained for microfluid
flow computations through the use of PDSMC. The capabilities of the developed parallel code are further demonstrated by the calculations of microfluid flows with heat transfer.

Parallel Implementation of DSMC

The conventional DSMC simulations describe the time-dependent evolution of the molecules. The solution for a steady state case is considered as an asymptotic limit of a corresponding unsteady flow. As the simulated molecules move, they collide with the other simulated molecules and interact with the physical boundaries. The locations and the velocities of these simulated molecules are determined and stored in sequences of time. Figure 14 is the conventional DSMC flowchart, showing the main procedures for a DSMC application. The core of the DSMC algorithm consists of four primary processes: particle movement, particle indexing and cross-referencing, collision simulation, and flow field sampling.

The conventional DSMC has been widely used for hypersonic rarefied gas flow calculations (Rault and Woronowicz 1995; Bird 1990; LeBeau 1999; Dietrich and Boyd 1995; Wilmoth and Carlson 1992). In Chapter 5, DSMC has been used in the predictions of the heat transfer characteristics of supersonic flows in microchannel (Liou and Fang 2001). In Chapter 6, an implicit treatment of the flow boundaries was developed for the DSMC of subsonic microfluid flows (Liou and Fang 2000). In contrast to the conventional “vacuum” boundary conditions, the implicit treatment accounts for the molecular fluxes across the flow boundaries due to local thermal motions. The local mean velocities, temperature, and number density at the
boundaries determine the number of the entering molecules, their velocities, and internal energies at every sample average step. The implicit treatment has been successfully applied to the simulations of micro-Couette flows and micro-Poiseuille flows. The detailed implicit boundary treatment has been described in Chapter 6. The DSMC code with the implicit boundary treatment is parallelized with the message passing interface (MPI) library (Gropp et al. 1994) and will be described in the following.

The present parallelization of the DSMC method is based on the single program, multiple data (SPMD) model. The physical domain is decomposed and each of its sub-domains, along with its associate cells and molecules, is allocated to an individual processor (see Figure 43). A complete DSMC code is loaded on to all processors and the simulation in a sub-domain proceeds independent of the other sub-domains at each time step. Information of the molecules that will cross the sub-domain boundaries during the movement portion of the DSMC algorithm is sent to the appropriate processor using MPI. Thus, the simulations are synchronized between the movement and collision routines at each time step. Since each processor contains a complete copy of the base simulation code, any addition to or modification of the base simulation algorithm to include, for example, a more complex geometry or collision physics can be readily implemented. In the following, the domain decomposition (data distribution) and the MPI communication model are described.

Data Distribution

The physical region of interest is decomposed into a set of sub-domains as
shown in Figure 43. The sub-domains are mapped onto different processors. For example, Figure 43 shows the sub-domain $\Omega_{i,j}$ and all of its neighboring sub-domains in a 2D space. The interface, which separates $\Omega_{i,j}$ from its neighbors, represents flow interface boundary. Molecules may move through the interfaces between $\Omega_{i,j}$ and the neighboring sub-domain during a time step. It is important to PDSMC that those molecules that exit $\Omega_{i,j}$ through the interface to one of its neighboring sub-domains should be registered and properly accounted for in their new “home” sub-domain and be deleted from the original sub-domain. In other words, there should be no loss/addition of molecules due to the decomposition of the flow domain.

Figure 43. Sketch of domain decomposition.

To this end, sending buffers are used in the present work. Each sending buffer is assigned to one of the neighboring sub-domains to store the information of the molecules that will travel to that particular sub-domain. For example, in the case of a
2-D flow as shown in Figure 44, the sub-domain \( \Omega_{i,j} \) has eight sending buffers. The outgoing molecules have, at the most, three possible sub-domains to go to through any flow interface boundary. At each time step, a molecule that is going to exit the current sub-domain after a full time step is dealt with by a "remove" procedure. The remove procedure determines the new home of the exiting molecule based on its location after the current time step. Since the future sub-domain where this molecule will reside has been found, the current information of the position, velocity, internal energy, rotational energy, gas species, and the remaining portion of the time step associated with this molecule can be saved in the corresponding sending buffer. The molecule is then taken out of its current sub-domain.

There are also molecules entering this sub-domain \( \Omega_{i,j} \) from its neighbors. This is not shown in Figure 43 for clarity. The information for the entering molecules is saved in respective receiving buffers after the data communication between the related processors has completed.

**Data Communication**

After the movement of all the simulated molecules and before the collision process can begin during each time step, all the processors must make necessary data-exchange of the information stored in the sending buffers described earlier. The communication between the processors proceeds with information on the number of molecules in transfer and their coordinates, velocity, rotational energy, and time step remaining. For data communication, there is an additional startup time needed for the
processors to be ready to transfer data. The startup time for data communication for PC clusters is much lengthier than that for other high-performance parallel architecture machines. In the present work, a new data type, \textit{msg\_mpi\_t}, is derived and all the data associated with the molecule crossing the flow interface boundary is transferred as a whole using this newly defined data type.

Inside this new data type, all the values are continuously distributed logically on a segment of RAM for each processor, so that they can be transferred as a whole using MPI. Therefore, this new data type is used as a template to send and receive data of the information of transferred molecules. Before the sending of the molecules, all the information is encoded into this template. And after the receiving, all the information is decoded back to a proper receiving buffer from the template.

While exchanging information between the processors, the processors must avoid sending data to or receiving data from each other at the same time. It is also important to be sure that the targeted processor receives the data that have been sent by another processor. Otherwise, it could cause a dead lock among the running processors. In this work, a synchronous communication model has been used for the \textit{myid}\textsuperscript{-th} processor, which calculates the \((\textit{myid}+1)\text{-th}\) sub-domain as shown in Figure 44.

The communication is followed by a procedure of “cross-move”, where the entering molecules stored in the receiving buffers are allowed to travel in the remaining time interval to reach their new positions. The newly arrived molecules can then be indexed into new grid cells. After this cross movement, the collision and
sampling average procedures proceed in the same manner as that of the conventional DSMC method. Figure 45 shows the flowchart of the PDSMC procedure implemented in this work. The additional steps used in the present implementation, in comparison with the conventional DSMC given in Figure 45, are enclosed in the dashed area.

MPI_Barrier make sure that all processors be ready to exchange data
To find the total number ii of its neighboring subdomains
do ith = 1, ii
   ip = the processor number of its ith neighboring subdomains;
   if (myid < ip) then
      copy data of the ith sending buffer to template of mesg_mpi_t;
      MPI_Ssend send mesg_mpi_t to processor ip;
   else
      MPI_Recv receive mesg_mpi_t from processor ip;
      copy the data of mesg_mpi_t to its receiving buffer;
   endif
endo
do ith = 1, ii
   ip = the processor number of its ith neighboring subdomains;
   if (myid > ip) then
      copy data of the ith sending buffer to template of mesg_mpi_t;
      MPI_Ssend send mesg_mpi_t to processor ip;
   else
      MPI_Recv receive mesg_mpi_t from processor ip;
      copy the data of mesg_mpi_t to its receiving buffer;
   endif
endo
do ith = 1, ii
   clear the ith sending buffer
endo

Figure 44. MPI synchronous communication model.
Parallel Machine

All the parallel computations referred to in this dissertation have been performed on the CEPCOM at the CFD laboratory in Western Michigan University.

Figure 46 is the front view of CEPCOM. CEPCOM is a 23-node Beowulf-class cluster assembled in September 2001. Each node has two 1GHz Pentium III processors and 512MB RAM. The machines are connected via the fast-Ethernet network, which can support up to 100Mbps bandwidth for each node. A HP ProCurve
Switch 4000M with a backplane speed of 3.8Gbps is used for the networking. All the processors are dedicated to run parallel jobs or high throughput jobs. The operating system is the Red Hat Linux 7.0. MPI library, *mpich-1.2.2*, is used for parallel programming in C/C++/Fortran77/Fortran90.

The overall peak performance of CEPCOM is 46 Gflop/s, with total of 11.5GB RAM and 302GB hard drive space.

Figure 46. Back view of CEPCOM.
Results and Discussions

The performance and efficiency of the PDSMC are examined using the microfluid flows in microchannels, which include a straight microchannel and a microchannel with a patterned surface structure.

Parallel Performance Benchmarking

A micro-Poiseuille flow has been calculated to benchmark the performance of the PDSMC code. The size of the microchannel is 5x1μm, with the computational grid of 400x80 uniform rectangular cells. The total number of the simulated molecules is about 1.6 million. The pressure ratio is 4.0. The microchannel is divided into multiple numbers of sub-domains of equal size and each sub-domain is assigned to a processor. The parallel calculation achieves a satisfactory load balancing and the total computing time decreases as the number of processors increases. Figure 47 shows a sketch of the domain decomposition for 32 processors. Figure 48 shows the variation of the total computing time for 400 iterations for a range between 1 and 32 processors. For such a problem, runs on a single Pentium III processor take nearly 2560 seconds, and for a 32-processor run, it is about 166 seconds. The speedup enhancement with the increasing number of processors is given in Figure 49. The speedup is defined as the ratio of the total computing time on one processor to that on multiple processors. It digresses away from the ideal linear variation at 8 processors, beyond which the communication time and synchronization overhead increase relatively to the calculating time on each processor for this problem of fixed size. The
speedup can be obtained up to 15.5 on 32 processors. Figure 50 shows the corresponding efficiency, which is defined as the ratio of the speedup to the corresponding number of processors used to run the problem. A nonlinear speedup is achieved within 8 processors. Especially on 2 processors, the efficiency of parallel computing is about 105%. Running on 32 processors, the efficiency can be kept within 48%.

Figure 47. Domain decomposition for a 2-D microchannel flow.

Figure 48. Total computing time for 2-D microchannel flow.
Figure 49. Speedup for a 2-D microchannel flow.

Figure 50. Efficiency for the 2-D microchannel flow.

From this simple benchmark, it can be seen that the parallel processing can clearly provide significant reductions in total computing times for DSMC.
calculations. And DSMC can be parallelized very efficiently to run on PC clusters, such as CEPCOM.

**Patterned Microchannel Flow**

Depending upon the specific application, the internal flow passage in MEMS may contain various forms of blocks and cavities. These patterns can be micromachined with surface etching that selectively removes materials using, for example, imaged photoresist as a masking template. Figure 51 shows a typical cross sectional view of such patterns. Compared with the micro-Couette and micro-Poiseuille flows simulated in Chapter 5, the flow inside the geometry of Figure 51 is highly two-dimensional. To examine the thermal and microflow phenomena in a more realistic geometry, the present PDSMC code is applied to simulate the microchannel flows with surface heating structure.

![Figure 51. Sketch of patterned microchannel.](image)

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The flow domain is divided into 10 sub-domains with boundary denoted by the dash lines. The computations were performed using 10 processors, with 16,000 uniform rectangular cells. The number of the simulated molecules is about 1.6 million. The inlet gas pressure is 0.73atm and temperature is 300K. For comparison, two cases with different exit pressure have been computed. The corresponding pressure ratios are 2.5 and 4.0 for Case 1 and Case 2, respectively. The channel height is 0.9μm with an aspect ratio of 6.7 and the block height is 0.3μm. The wall temperature is 323K, except for the top of the blocks with a temperature of 523K. The Knudsen number, based on the inlet conditions, is about 0.08. Runs of 200,000 time steps, with sampling after 2,000 time steps of development take roughly 48hrs. The computed results are shown in the following.

Figure 52 shows the contours of pressure for both cases. There is a more significant variation of pressure in the streamwise than in the transverse directions. The difference in the pressure drop between the two cases becomes more distinguishable in the latter half of the microchannel. Figure 53 shows the pressure distributions on the top and bottom wall for both cases. Except for the regions near the blocks, the wall pressures vary almost linearly in the streamwise direction.

Figure 54 shows the density contours in the microchannel for the two cases. The contours are seen to continue smoothly across the boundary of the sub-domains, suggesting a successful implementation of the parallel algorithm described above.
Figure 52. Pressure contours.

Figure 53. Pressure distributions on the upper and lower wall.
Figure 54. Density contours.

Figure 55 shows the contours of the magnitude of the streamwise velocity component $u$. Again, the flows are seen to develop in a rather continuous manner across the interfaces between the sub-domains. As expected, higher-velocities can be observed in the regions above the blocks. Figure 56 shows the streamwise distributions of $u$ at three different vertical locations; one at the midway between the top of the blocks and the top wall, the second at the top of the blocks, and the third at one half of the height of the blocks. The distributions are quite smooth and no apparent discontinuities can be observed across interfaces. It suggests that sufficiently high resolution has been achieved in the PDSMC simulations and the statistical error is small in the present microchannel simulations of near-atmospheric pressures. It is shown that the streamwise velocity accelerates above the blocks and reaches its maximum near the end of the second block. The streamwise velocity at the exit for
Case 2 is about 108m/s, which is about twice of that for Case 1, due to the higher pressure ratio in Case 2. A phenomenon associated with high-$Kn$ flows is the slip velocity on the wall. Figure 57 shows the velocity-slip on the upper and the bottom wall. The distributions are similar to that of the streamwise velocities at the corresponding “Top-Mid” and “Mid-Step” locations in Figure 56. Figure 58 shows the transverse velocity distributions along the same heights as those of Figure 56. The flows become increasingly more two-dimensional as they develop down-stream, indicating a fair amount of convective mixing of both momentum and heat.

![Streamwise velocity magnitude contours](image)
Figure 56. Streamwise velocity distributions.

Figure 57. Velocity slip along the upper and lower wall.
Figure 58. Transverse velocity distributions.

Figure 59 shows the temperature contours for both cases. Mushroom-like regions of high temperature can be observed surrounding the blocks, due to the high temperature at the top of the blocks. These high temperature regions for the two cases are geometrically similar. Figure 60 shows the streamwise variation of temperature at two height levels for both cases; one at the top of the blocks and the second at midway between the top of the blocks and the top wall. The temperature in the regions above the blocks is significantly higher than the regions upstream and downstream of the blocks. The highest temperature change is roughly 60K between these two levels, which are 0.3 µm apart. Except for the region above the second block, there is a minimal difference in the streamwise temperature distributions between the two cases.
Figure 59. Temperature contours.

Figure 60. Temperature distributions.
Figure 61 shows the temperature-jump distributions along the upper and the horizontal part of the lower walls. The temperature-jumps along both the upper and the lower walls are high in the regions around the blocks. The absolute value of the temperature-jump is higher on the top surface of the block than on the upper wall. For instance, on the top surface of the first block the temperature-jump is nearly 80K, while that for the upper surface is about 20K. Overall, the temperature-jump distributions for Case 3 are similar to those of Case 4. A comparison of the heat transfer at the top channel wall for the two cases is given in Figure 62. The peak values roughly correspond to the locations of the blocks. The heat transfer for the low pressure-ratio case (low Kn) is slightly higher than that for the higher value. This agrees well with the results for the micro-Poiseuille flows presented above where the flow with high Kn shows less heat transfer compared to that with lower Kn.

Figure 61. Temperature-jump on the upper and lower wall.
Concluding Remarks

The implementation of a new parallel algorithm for DSMC has been described. The performance and efficiency of the parallel DSMC algorithm have been demonstrated through simple benchmarking of a micro-Poiseuille flow. Applications of the code to simulate a patterned microchannel flow have been presented. The results show that the parallel algorithm can provide significant reductions in total computing time for DSMC calculation, and DSMC can be parallelized efficiently for cluster computers, such as the CEPCOM.

The results of the patterned microchannel flow show that the Knudsen number and the geometric complexity of the channel have significant effects on the fluid dynamic and the thermodynamic behavior of the microfluid flows studied.
CHAPTER VIII

PARALLEL DSMC SIMULATIONS OF CHAOTIC MICROFLOWS

Introduction

While the problems of the instability of laminar flows and their transition to turbulence have been studied for a long time in classical hydrodynamics, the corresponding problems in kinetic theory have also received much attention recently (Cercignani 2000). The study of such problems might be of great importance for the purpose of understanding fundamental phenomena of flow instability and self-organization from first principles.

During the past decade, the DSMC method 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 (Riechelmann and Nanbu 1993; Stefanov and Cercignani 1993). The Taylor vortices were observed for a range of Kundsen numbers in these two-dimensional (axisymmetric) flow computations. The convective instability associated with the Bernard cells has also been studied (Stefanov and Cercignani 1992).

In most of these studies, steady flows were of interest and calculations were conducted to achieve stationary states of the calculated flow. The computations are usually two-dimensional or axisymmetric. However, DSMC allows for a direct
physical simulation of gas flows by nature of its design. A minimum level of physical modeling is needed at the level of molecular models that have been used in the kinetic theory of gases. The work reported here represents an effort to take advantage of this largely unexplored characteristics of DSMC and to apply the method to simulate the time-dependent behavior of gaseous flow. Such first principles simulations are useful in obtaining a detailed fundamental understanding of the physical mechanisms at work in many fluid flow phenomena, such as transition and turbulence at high speeds.

The flow model considered is a micro-Couette type of flow with an imposed artificial forcing (AF). The flow geometry considered is shown in Figure 63. The flow develops between two diffuse walls in the y-direction; the top wall moves at a speed of $U$ in the x-direction at zero time. The lower wall is stopped instantaneously at the beginning of the calculations. Periodic boundary conditions are applied in the x- and z-directions. An artificial gravitational forcing is applied to the molecules along the y-direction in the micro-Couette flow, which is proportional to the square of the difference between the local macroscopic flow instantaneous velocity component in the moving direction of the top surface and the magnitude of the surface velocity. In other words, the AF is proportional to the square of the macroscopic velocity deficit.

$$AF = a(\hat{u} - U)^2$$  \hspace{1cm} (8.1)

A similar geometry with an imposed acceleration has previously been employed (Malek Mansour 1990) to study analytically the onset of instability. It is not the aim of the present study to examine the centrifugal instability problems. We seek to verify, by taking advantage of the recent advances of parallel computing, that DSMC
can be used to simulate the formation of vortical structures in three-dimensional flows in a time-dependent manner.

Figure 63. Flow geometry for chaotic flow.

With the forcing described in equation (8.1), when a fluid particle is perturbed and moves in the $y$ direction, the artificial gravitational buoyant force further displaces the particle in the $y$-direction. The scenario is similar to the instability mechanism associated with the centrifugal force in the Taylor-Couette and Gortler problems, in which Taylor-Gortler vortices have been observed in experiments and computed by using two-dimensional DSMC. Given the similarity between the artificial forcing of equation (8.1) and the centrifugal force, it is reasonable to expect that the current time-dependent simulations will also exhibit vortical structures or flow patterns in certain steady-state solutions. The use of an artificial forcing, instead of a physical one, allows direct control of the level of forcing and a total switch-off, when it is desired, to study the decay of the vortices generated by the forcing.
As the DSMC method is based on a molecular description of gases, there have been concerns (Meiburg 1986) 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. (1988) show that as long as the cell size is sufficiently small, the total angular momentum is nearly conserved. Bird (1987b) has also shown that the non-conservation of the angular momentum has no significant effects on the DSMC solutions, provided that the collision partners have a mean separation distance that is less than the local mean free path.

As a large number of particles are required in a DSMC simulation to reduce the inherent statistical scatter, the computer resource needed to perform time-dependent, three-dimensional flow simulation can be significant. This appears to be a major limiting factor for performing many necessary three-dimensional simulations. The simulations presented here have been performed by using the developed parallel DSMC algorithm (Fang and Liou 2002b) described in Chapter 7 on a parallel computer cluster CEPCOM in the CFD Laboratory at Western Michigan University.

Parallel DSMC Program for Chaotic Microflows

The scheme that is outlined in the introduction has been implemented in a dedicated three-dimensional PDSMC program called SCFMPI for “strong chaotic flows coded with MPI library”. For simplicity, the HS molecule model is used for the elastic binary collision process. In the gas-surface interaction, the Maxwellian diffuse reflection model is considered. This program employs non-dimensional variables with
distances normalized by the mean free path in the initial gas $\lambda_0 = 1/((\sqrt{2\pi d^2})^n)$. A Knudsen number is defined as the ratio of $\lambda_0$ to the distance $h$ between the lower and upper boundaries so that the distance is effectively the inverse Knudsen number of the flow. Temperature and density are normalized by their values in the initial gas. Velocity is normalized by the most probable speed of molecules in the initial gas, $c_{mp}$. And the physical flow time $t$ is normalized by the mean collision time of molecules in the initial gas, $t_{c,0}$. That is, $t = t^* t_{c,0}$, where $t^*$ is the normalized computational time in DSMC and $t_{c,0} = (\sqrt{\frac{\pi}{2}}/\sqrt{T_0})(\lambda_0/\sqrt{2R})$ for HS molecule model. A convenient macroscopic reference time is the time in which the surface or flow at the upper boundary moves a distance equal the distance between the lower and upper boundaries and it is $h/U$. For the HS molecule model, the ratio of the physical time to this reference time, $tU/h$, can be expressed as

$$\frac{tU}{h} = \frac{\sqrt{\frac{\pi}{2}} t^* U^*}{h^*}$$

(8.2)

where the superscript * denotes the non-dimensional value with $U^* = U/c_{mp}$ and $h^* = h/\lambda_0$.

In order to improve the DSMC efficiency and accuracy, the transient sub-cells (Bird 1999) is used in the SCFMPI, which is much like the static sub-cells introduced in Chapter 3. The transient rectangular sub-cells are generated for one flow field cell at a time within the collision routine. The molecules are then indexed to these transient sub-cells. The size of sub-cells is set such that there are approximately two simulated molecules within each sub-cell element. The variables for the transient sub-
cells are allocated when the number of cell molecules is decided and are deallocated when the collisions have been calculated for the flow field cell. The first molecule for a potential collision is chosen at random from the cell. The transient sub-cell in which it lies is determined from the indexing and, if there is more than one molecule in the sub cell, the collision partner is chosen from this sub cell. If there is only one molecule in this sub-cell, the collision partner is chosen from an adjacent sub-cell. The access to the adjacent sub-cells is random in order to avoid artificial correlations in the location of collision partners. This yields nearest neighbour collision and is efficient with regard to both computation time and storage requirements. The ratio of the mean separation between collision partners to the local mean free path should be well under unity over the flowfield.

The flow properties are sampled on both an unsteady and a time-averaged basis. In the unsteady case, an instantaneous property of macroscopic flows, for instance, the vertical velocity $\hat{v}$ at time $t$ is the average of its corresponding molecular property over a short time $t_\tau$; i.e.,

$$\hat{v} = \frac{1}{t_\tau} \int_{-\frac{1}{2}t_\tau}^{\frac{1}{2}t_\tau} \sum_{i=1}^{M_c} c_{vi}(t') dt'$$

(8.3)

where $c_v$ is the vertical component of the molecule velocity, and $M_c$ the molecule number in the flow field cell averaged at time $t'$. In the time average case, the sampling can be reset at any time and the variable $v$ is called the mean property of macroscopic flows, which is the time average from the reset time $t_0$ to its current time $t$; i.e.,
Then the relationship between the instantaneous property and the mean macroscopic property can be expressed as

\[ \tilde{v} = v + v' \]  

(8.5)

where \( v' \) is the perturbation of variable \( v \) at time \( t \).

All the calculations in this chapter are for the upper surface moving with a speed \( U \) in the \( x \)-direction. The gas molecules are initialized uniformly with a mean velocity as of the upper surface and the disturbance spreads from the lower surface. The uniform flow option would be valid only up to the time that the disturbance reaches the upper boundary. SCFMPI is a three-dimensional code. If a single computational cell is set in the \( x \)-direction, the two-dimensional flow in the \( y \)-\( z \) plane may be studied. This is referred to as the transverse mode. Similarly, the two-dimensional longitudinal mode in the \( x \)-\( y \) plane may be studied by setting a single cell in the \( z \)-direction.

In the transient sub-cell scheme, each direction of the field cell is divided into 10 equal elements, such that there are \( 10^3 \) sub-cells in every flow field cell for three-dimensional problems and \( 10^2 \) sub-cells for two-dimensional problems. The time step is set to 0.2 times the molecular mean collision time in the initial gas. That is, \( \Delta t_d = 0.2t_{c_0} \) and \( \Delta t^* = 0.2 \). In the unsteady sampling, the short time period is set to 20 times the molecule mean collision time in the initial gas \( (t_s = 20t_{c_0}) \).

As a large number of particles are required in the forced chaotic flow...
simulations to reduce the inherent statistical scatter, the computer resource needed to perform time-dependent, three-dimensional flow simulation is significant. SCFMPI has been implemented by using the parallel algorithm (Fang and Liou 2002b) for DSMC described in Chapter 7. Figure 64 shows the flowchart of the SCFMPI implementation, where the left half part is for the DSMC procedures for unsteady flows, and right half part is for the procedures to parallelize this unsteady DSMC algorithm. Compared with Figure 45, there are extra procedures for the unsteady sample average and the calculation of flow property perturbations for the conventional DSMC methodology, and the implicit boundary conditions have been changed to periodic boundary conditions.

![Flowchart of the SCFMPI implementation]

Figure 64. Flowchart of the SCFMPI implementation.
Simulation Results and Discussions

In this section, the results of the present PDSMC simulation for a two-dimensional slice of the model flow geometry are first compared with independent serial calculations. Results for two- and three-dimensional simulations of the model flow are presented.

The flow simulated has the top wall speed \( U \) set equal to the most probable molecular speed at the initial gas temperature of 1,000K. Monatomic, non-reactive gas is assumed. The HS model and the diffuse wall boundary conditions are used for the collision process.

Two-Dimensional (2D) Simulations

The parallel DSMC code used in this study has been validated by comparing it with the results for microchannel flows (Liou and Fang 2000) and is reported in Fang and Liou (2002b). For the present flow geometry, comparisons have also been made with the serial code results of Bird for a 2D domain that slices through the current model flow along a \( z \)-plane. These are comparisons of the longitudinal mode. The size of the computational domain in the \( x \) - and the \( y \)-direction is 180×60, nondimensionalized by the initial mean free path \( \lambda_0 \). The Knudsen number \((Kn)\) defined by the channel height \( h \) is then 1/60. The field cell size is 90×30, and two million molecules are simulated. The value of \( a \) in the artificial gravitational force formula is 0.1. The forcing is equivalent to a centrifugal forcing corresponding to a radius of ten mean free path of the initial gas. Figure 65 shows comparisons of the
vertical velocity perturbation contours and the pathlines between Bird's results and
the present parallel DSMC results after the simulated flows appear to have reached a
periodic flow pattern. As defined in equation (8.5), the perturbation velocity
component, say the vertical component $v$, is defined as the difference between the
"unsteady" sample average $\bar{v}$ that is taken over a short time interval and the long
time-averaged $v$. The results of the parallel runs using two different types of domain
decomposition are shown: 1DD denotes one-directional decomposition and 2DD two-
directional. Small statistical scatter can be observed in all three results. The pathlines
show that the overall flow patterns are basically the same, both capturing a small
region of vortical flows at the heel of the region of large, positive vertical velocity
perturbation. Similar contour patterns are also observed in the 2DD results. Note that
the boundaries are periodic and it is difficult to time the outputs so that comparable
flow patterns appear at the same location for all three plots in Figure 65.

The results shown in Figure 65 indicate that the length of the domain, 180,
might be too small to contain more than one cyclical flow pattern. A series of 2D
cases with larger domains was examined. Figure 66 shows the vertical velocity
perturbation contours and pathlines for a case with $1200 \times 100$ cells, $a = 0.04$, and 8
million computational molecules. There are three identifiable periodic flow patterns.
The flow patterns are quite regular, with a wavelength $\Lambda$ of about 400, and are rather
smooth. In time, the cyclic flow pattern moves in the $x$-direction. Figure 67 shows the
evolution of the instantaneous specific kinetic energy averaged over all the cells
defined as
Figure 65. Comparisons between parallel and serial DSMC results for vertical velocity perturbation contours and pathlines.

Figure 66. Vertical velocity perturbation contours and pathlines at $tU / h = 326$. 

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where the summation is applied to all the flow field cells and \( N \) denotes the total number of cells. The kinetic energy settles after an initial transient to finite amplitude oscillations. A part of the curve in the region of the finite amplitude oscillations has been enlarged and is also included in Figure 67. These curves show that the averaged kinetic energy varies quite regularly and the flow has essentially reached a quasi-periodic state after 1,000 print cycles, or 20,000 initial mean molecular collision time, \( t_c \). It can be seen from Figure 66 that the flow associated with the quasi-periodic state features flow structures with wavelength of about 400. Before the quasi-periodic state is reached, the simulated flow continuously evolves in time as it develops from the initially chaotic flow. The region near the bottom wall is strongly rarefied and first shows significant patterns of small-scale variations. As time advances, some small-scale patterns amalgamate and grow and others decay after their initial generation. Figure 68 shows the pathlines of flow disturbance at different time, \( tU/h = 21.8, 56.3 \) and 123.1 for (a), (b) and (c), respectively, when the flow is in transition from the initial chaotic to the quasi-periodic states. Vortices of different sizes can be identified; some span across the height of the channel. Some vortices are formed at first, and then amalgamated and reorganized to larger and much more patterned vortices. These vortices are unstable. The flow eventually evolves into a regular disturbance pattern as is shown in Figure 66 for \( tU/h = 326 \).
Figure 67. Evolution of the instantaneous cell-averaged kinetic energy.

Figure 68. Pathlines of the flow disturbance with $h=100$ at different time. (a): $tU/h = 21.8$; (b): $tU/h = 56.3$; (c): $tU/h = 123.1$.

The distribution of the vertical velocity perturbation along the $x$-direction for $y = 66$, at time $tU/h = 326$ when the flow has become quasi-periodic, is shown in
Figure 69. The three concentrated regions of high, positive vertical velocity perturbations are associated with the three cyclical flow patterns in Figure 66. The wavelength is about 400. The signals associated with the dominant flow pattern with wavelength 400 are quite smooth with little statistical scatter. In between, there appear to be waves of smaller wavelengths. The Fourier wave number spectrum of the vertical velocity perturbation signal given in Figure 69 (along \( y = 66 \)) is shown in Figure 70. The Fourier spectrum of the initial, chaotic state has also been included for comparison. At the high wave number end, the spectrum is filled with low amplitude noise, as can be expected from a statistical simulation such as DSMC. At the low wave number end, multiple discrete peaks with amplitudes one to two orders of magnitude higher than those at the high wave number end appear. The first peak, with a wave number of 3, has a wave length of 400, corresponding to the flow pattern described earlier in Figures 66 and 69. The next peak has a wavelength of 400/2. If one refers to the wave with a wavelength of 400 as a fundamental mode, the wave with a wavelength of 400/2 is then its first harmonic. In all, about nine or more higher harmonics can be identified in Figure 70 before their amplitudes drop off. Since neither the applied forcing nor the initial flow contains any preferred time and length scales, the generation of these harmonic waves is not associated with any externally imposed excitation, which is often applied in Navier-Stokes-based flow simulations. The wave hierarchy appears in the current DSMC simulations as a result of the nonlinearity of the simulated flow.
Figure 69. Distribution of vertical velocity perturbation along $y = 66$. $tU/h = 326$.

Figure 70. Fourier wave number spectrum of the vertical velocity perturbation along $y = 66$. $tU/h = 326$.

Figure 71 shows the time-dependent evolution of the Fourier amplitudes of four wave numbers, with $n = \alpha/3$. They are associated with the first three harmonic
waves and a high wave number mode (n=60). The harmonic modes arise from the initially chaotic flow and grow in amplitude as the flow develops. They then become quasi-periodic at large time. At high wave number (n=60), the mode was initially amplified but becomes subdued with time. As the applied forcing is artificial, the growth of the harmonic waves and the resulting flow patterns may not be physically realistic. The results nevertheless show that DSMC can resolve a hierarchy of waves of a fundamental mode with wavelength $A = 400$ and its harmonics ($A = 400/n$).

![Figure 71. Time-dependent evolution of the Fourier amplitudes for the vertical velocity perturbation along y=66.](image)

As was noted earlier, the assumed forcing is similar to that of a centrifugal force and the Taylor-Görtler type of vortical motion is expected to be found in certain
steady state solutions of the current time-dependent simulations. 2D simulations for a plane in the $x$-direction have been performed. The flows are analogous to the two-dimensional Taylor-Couette problem. Figure 72 shows the time-averaged pathline patterns for a case where vortices similar to that of the Taylor-Gortler vortices are observed. The computational domain size as shown is $60 \times 180$ in the $y$- and $z$-directions, respectively. The flow appears to be steady. The pathlines are based on an average from $tU/h = 24$ to $62$. The flow pattern indicates a regular vortical flow almost identical to that of the Taylor-Couette flows, and shows that the current time-dependent DSMC is capable of capturing the Taylor-Gortler type of vortical flow motions.

Figure 72. Steady flow pathlines. $Kn=1/60$

The Knudsen number is $1/60$ for the flow in Figure 72. The flow patterns change as the Kundsen number decreases. The flow becomes varying with time and unsteady sampling must be used. Figure 73 shows the pathline patterns for two cases with $Kn=1/240$ and $1/500$, respectively. The corresponding domain sizes are $240 \times 720$ and $500 \times 1,500$. Compared to the vortical flow shown in Figure 72 ($Kn=1/60$), the numbers of identifiable vortices in Figure 73a for $Kn=1/240$ are the same and the vortices still span across the entire height of the channel. The vortices in Figure 73a,
however, are deformed and irregular. With a further decrease of the Knudsen number, Figure 73b (Kn=1/500) describes a flow pattern that is irregular and contains vortices of different sizes that form and decay as time develops.

![Flow pathlines. (a) Kn=1/240, tU/h =20; (b) Kn=1/500, tU/h =13.](image)

The 2D simulations performed on the two different cross-sectional cuts of the three-dimensional model flow have provided valuable insights regarding the applicability of DSMC to simulate time-dependent flows. They also serve as a guide to three-dimensional simulations, which are significantly more demanding on computational resources.

Three-Dimensional (3D) Simulations

Two 3D chaotic flows have been simulated with conditions shown in Table 8. In Case 1, an artificial forcing of $a = 0.04$ is applied to the three-dimensional model flow. The channel height is 60 and the Knudsen number is 1/60. The size of the computational box is $800 \times 60 \times 320$. The number of computational molecules is 16
million and the total number of uniform cells 320K. A total of 8 processors were used and the run time for the results shown was 11 days. Figure 74 shows the time history of the cell-averaged specific kinetic energy on an x-plane located at x= 400. After an initial transient, the flow appears to have become stationary and the statistical oscillations are small, as is shown in the insert in Figure 74. Figure 75 shows the In-plane pathlines and vorticity contours of the long-time average flow on the x-plane location at x=400 at time $tU/h = 11.8, 29.5, 76.7$ and 502 for (a), (b), (c) and (d), respectively. Three pairs of counter-rotating vortices were formed with different size at $tU/h = 11.8$ from the initial chaotic state, and the vorticity of the vortices was weak. With the increase of vortex vorticity, these vortices reorganized to four counter-rotating pairs at $tU/h = 29.5$. At time $tU/h = 76.7$, these four pairs of vortices evolved to three and half dominating pairs, with vorticity increased for the middle five vortices. Three regular pairs of vortices are further formed with almost equal vorticity and size as shown in Figure 75d at time $tU/h = 502$.

Table 8

| Three-Dimensional Chaotic Flow Simulation Cases and Conditions |
|---|---|---|
| Case 1 | Case 2 |
| Size ($\lambda_0$) | 800×60×320 | 800×320×640 |
| Forcing $\alpha$ | 0.04 | 0.04 |
| $U$ ($c_{mp}$) | 1.0 | 1.0 |
| $T_w$ (K) | 1000 | 1000 |
| Field cells | 200×20×80 | 200×32×64 |
| Time step $\Delta t^*$ | 0.2 | 0.2 |
| Molecules | 16 million | 48 million |
| Re | 108 | 578 |
| $1/Kn$ | 60 | 320 |
Figure 74. In-plane evolution of cell-averaged specific kinetic energy, at $x=400$.

Figure 75. In-plane pathlines and vorticity contours of the long-time average flow with $x=400$ at different time. (a): $tU/h = 11.8$; (b): $tU/h = 29.5$; (c): $tU/h = 76.7$; (d): $tU/h = 502$. 

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Figure 76 shows the distribution of the long-time averaged spanwise velocity at time $tU/h = 656.8$, along the middle of three $x$-planes located at $x/L = 0.1$, 0.5 and 0.9, respectively. The distributions are rather smooth. The cyclic distributions reflect the vortex pairs observed in Figure 75d. Figure 76 also shows that the simulated flow is nearly homogeneous in the $x$-directions, since there is not much difference among the velocity distribution of three $x$ locations. Figure 77 shows the Fourier wave number spectrum of the long-time averaged spanwise velocity distribution shown in Figure 76. At the high wave number end, the spectrum is filled with low amplitude noise. At the low wave number end, multiple discrete peaks with amplitudes two or three orders of magnitude higher than those appear at the high wave number end. The first peak, with a wave number of 3, has a wavelength of 107, corresponding to the fundamental mode of the flow pattern described in Figure 75d and Figure 76. Similar to Figure 70 of 2D case, the next peak has a wavelength of $107/2$ is the first harmonic of the fundamental mode. Two obvious harmonics can be identified in Figure 77 before their amplitudes drop off. Figure 78 shows the time-dependent evolution of the Fourier amplitudes of four wave numbers for the long-time averaged spanwise velocity in the middle of $x$-plane at $x/L = 0.5$. They are the first three harmonic waves and a high wave number mode ($n=12$). The harmonic modes, especially the first two harmonic modes, arise from the initially chaotic flow and grow to a nearly constant in amplitude as the flow develops; that is, the flow becomes stationary at large time. As the applied forcing is artificial, the formation of the flow patterns may not be physically realistic. But the results show that DSMC has the ability to capture a
hierarchy of waves of a fundamental mode for the second flow in a 3D problem.

Figure 76. Distribution of the long-time averaged spanwise velocity along the middle of x-planes located at $x/L=0.1$, 0.5, and 0.9, respectively. $tU/ h = 656.8$.

Figure 77. Fourier wave number spectrum of the long-time averaged spanwise velocity along the middle of x-planes located at $x/L=0.1$, 0.5, and 0.9, respectively. $tU/ h = 656.8$. 

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Figure 78. Time-dependent evolution of the Fourier amplitudes for the long-time averaged spanwise velocity in the middle of $x$-plane at $x/L=0.5$.

Figure 79 shows the pathlines on three planes at different $x$ locations at $tU/h=656.8$. Note that the top wall at $y=60$ moves along the $x$-direction. The pathlines indicate that a fluid flow exhibiting pairs of counter-rotating vortical motion may exist in the 3D simulation, a characteristic of the Taylor vortices.

Note that the results of the 2D transverse-mode simulation of the same Knudsen number also shows similar patterns of vortices. The value of $a$ is 0.1 in the 2D transverse-mode case. Figure 80 shows the contours of the time-averaged vertical velocity in the three planes perpendicular to the coordinate axes, respectively, at $tU/h=656.8$. The contour pattern in the $y$-plane shows streamwise streaks indicating that the vortical motions exhibited in Figure 79 are indeed imprints of pairs of counter rotating streamwise structures, or the Taylor vortices.
Figure 79. In-plane pathlines of the long-time averaged flow located at $x/L=0.1$, 0.5 and 0.9, respectively. $tU/h = 656.8$.

Figure 80. Contours of the long-time averaged vertical velocity on three orthogonal planes. $tU/h = 656.8$. 

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Figure 81 shows the in-plane pathlines in the three planes perpendicular to the coordinate axes, respectively, at $tU/h = 656.8$. The pathline pattern in the $z$-plane shows that the pathlines spread out from the region near the upper wall and swept in from the region near the lower wall from upstream to downstream. The tangent of the pathlines crossing a constant $y$-line is nearly parallel. The pathlines in the $y$-plane either bundle up underneath the regions of high positive vertical velocity or spread out underneath the region of high negative vertical velocity. The points to bundle up or spread out almost fall into six lines from upstream to downstream. These characters of pathlines in $z$- and $y$- planes show the flow is homogeneous in $x$-direction. The pattern suggests that fluid is swept in from the side and ejected upward in the up-wash part of the Taylor vortex motion. Similarly, the fluid is pushed downward and spread out sideways near the wall in the down-wash part of the Taylor vortex motion.

![Figure 81. In-plane pathlines on three orthogonal planes, color-coded by the magnitude of the long-time averaged vertical velocity. $tU/h = 656.8$.](image-url)
Figure 82 shows the Fourier spectrum of the long-time averaged specific kinetic energy where $K$ represents the magnitude of the 3D wave number vector, and $|e|$ the Fourier amplitude. At the low wave number end, the spectrum is dominated by a number of discrete peaks, each apparently corresponding to the coherent vortical flow pattern shown in the previous figures. Beyond $K=10$ at the higher wave number end, the spectrum shows, in general, a monotone decrease. The magnitudes are orders-of-magnitude smaller than the spectral peaks in the low wave number range, which are associated with identifiable flow signals.

Figure 82. Fourier wave number spectrum of the long-time averaged specific kinetic energy. $tU/h = 656.8$. 

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In all the simulations, the time step is set as 0.2 times the molecular mean collision time; i.e., \( \Delta t^* = 0.2 \). In order to validate the time step effects on the simulation accuracy, this case has also been run with a half-finer time step and the same unsteady sampling time period. That is, \( \Delta t^* = 0.1 \) and \( t^* = 20 \). Figures 83a and 83b show the instantaneous velocity evolution simulated with different time step at the field point (400, 30, 160), with \( \Delta t^* = 0.2 \) and 0.1 for 21a and 21b, respectively. There is no significant difference for both solutions. The corresponding mean velocity evolutions are also compared in Figure 84, and there is no significant difference, either. Therefore, the time step \( \Delta t^* = 0.2 \) is accurate enough to be used to simulate the chaotic flows in this chapter.

Figure 83a. Instantaneous velocity evolution at (400, 30, 160) with time step \( \Delta t^* = 0.2 \).
Figure 83b. Instantaneous velocity evolution at (400, 30, 160) with time step $\Delta t^* = 0.1$

Figure 84. Comparison of the mean velocity evolutions at (400, 30, 160), with time step $\Delta t^* = 0.2$ and $\Delta t^* = 0.1$
In Case 2, the size of the computational box is increased to 800\times320\times640. The inverse Knudsen number is 320. The top wall velocity, the temperature on the walls and the artificial forcing remain unchanged. The Reynolds number, based on the channel height and the initial flow quantities, is about 578.

The data presented in Figure 85 show the long time-average in-plane streamlines for four different times $tU/h$, and for three axial locations. The long time-average of the flow begins at the initiation of the simulations. At the nondimensional time, $tU/h = 7.5$, the average flow shows the formation of vortices of different sizes from a chaotic initial flow due to the applied forcing. In contrast to the regular vortices observed in Figure 72 for the case with $h=60$, the size and the shape of the vortices vary significantly. The flow is also far from being homogeneous in the streamwise direction. The flow develops further at later times. The vortices appear to deform in different ways. Some grow as they merge with the neighboring ones. New regions of vortical motion can also be identified. Since these are in-plane streamlines, the appearance of a convergence to a point in a streamline indicates a strong fluid motion in the third direction, the $x$-direction in this case. At $tU/h = 16.8$, a large vortices forms near the periodic boundaries in the $z$-direction. The centerline region is occupied by two connected vortices. Some small vortices seen in the earlier time have disappeared. At $tU/h = 20.1$, the flow pattern is still developing for all three planes shown. While merging of vortices can be observed in some parts of the flow, new small-scale vortical motions are also generated. After nearly 5,000 unsteady-sampling time periods, the flow appears to be still developing.
Figure 85a. In-plane streamlines of long time-average flow with $h=320$, at $tU/h=7.5$.

Figure 85b. In-plane streamlines of long time-average flow with $h=320$, at $tU/h=10.8$. 

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Figure 85c. In-plane streamlines of long time-average flow with $h=320$, at $t_{U/h}=16.8$.

Figure 85d. In-plane streamlines of long time-average flow with $h=320$, at $t_{U/h}=20.1$.

Figure 86 shows the kinetic energy spectrum of the long time-average flow at
$tU/h = 20.1$. Compared with the energy spectrum for the case with $h=60$, discernable peaks appear in the high wave number end, indicating the existence of motions of smaller length scales.

![Energy Spectrum](image)

Figure 86. Kinetic energy spectrum of the mean flow with $h=320$, at $tU/h=20.1$.

Figure 87 shows the in-plane streamlines of the disturbances at $tU/h=20.1$. It bears little resemblance to that for the long time-average. Figure 88 shows the spanwise distributions of the spanwise disturbance velocity at three axial locations at $tU/h=20.1$. Compared with Figure 76, the spanwise velocity distributions do not exhibit any apparent regularity in both the spanwise and the streamwise directions. Figure 89 shows the FFT of the three signals given in Figure 88. The spectrum does not show discrete mode dominating the spanwise disturbances.
Figure 87. In-Plane streamlines of the disturbance flow with $h=320$, at $tU/h=20.1$.

Figure 88. Spanwise disturbance velocity of the flow with $h=320$, at $tU/h=20.1$. 
Figure 89. FFT of Spanwise disturbance velocity for the flow with $h=320$, at $tU/h=20.1$.

Figure 90 shows the disturbance kinetic energy spectrum at $tU/h=20.1$. The spectrum is quite full at the low wave number end, indicating that the disturbance motions contain no dominant discrete modes.

Figure 90. Kinetic energy spectrum of the disturbance flow with $h=320$, at $tU/h=20.1$.
Concluding Remarks

The DSMC method has been applied to study the time-dependent behavior of an initially chaotic Couette flow. Two-dimensional and three-dimensional geometries were studied. The results show that the applied artificial forcing drives the flow into organized patterns, similar to that observed in the Taylor-Gortler problems. Vortical structures have also been identified that are associated with a hierarchy of waves, consisting of a fundamental mode and its harmonics. Despite the fact that the forcing amplitude may be unrealistic, the results of the simulations show that the particle-based DSMC method has the capability to capture the nonlinear evolution of harmonic waves, which is generally recognized as a necessary route that precedes laminar breakdown. This finding, we believe, has not been reported in the open literature.

The results for the limited window of parameters presented in the paper suggest that DSMC can capture important flow phenomena and can be a viable computational tool for time-accurate high-speed flow simulations. There are other important parameters for the model flow problem that require further studies. This would include, among others, the flow conditions, the collision models, Knudsen numbers and the imposed gravitational forcing.
CHAPTER IX

MICROFLOW AND HEAT TRANSFER SIMULATIONS BY BURNETT EQUATIONS

Introduction

For many fluidic MEMS, the characteristic dimension of the flow, \( h \), is comparable to the mean free path of the fluid, \( \lambda \). Under such conditions, the "continuum hypothesis", which is the underlying principle for the scaling laws developed for large geometry, is no longer valid. In general, the breakdown of the continuum hypothesis occurs, say, when \( Kn > 0.1 \). For such flows, the Navier-Stokes equations are inadequate, since the equations are developed for flows with small deviations from local thermodynamic equilibrium. The Knudsen number for the flows in MEMS can be larger than 0.1, indicating that the flow in MEMS lies in the continuum-transition regime. The main computational approaches that can be used for fluid flows in such continuum-transition regime, such as microfluidic flows, include the DSMC method and the Burnett-equations-based CFD method.

The DSMC approach, which simulates the gas flow from a molecular point of view, is an effective and robust tool for the continuum-transition flows (Liou and Fang 2000, 2001; Fang and Liou 2001). Its main disadvantage is the large requirement for computer memory and CPU time. This is especially true when the flow
approaches the continuum limit. Therefore, the DSMC is an appropriate method for microchannel flows with large Knudsen numbers and becomes computationally expensive as the Knudsen number decreases.

Constitutive relations for a gas near thermodynamic equilibrium can be derived as approximate solutions of the Boltzmann equation using the Chapman-Enskog expansion. This method yields constitutive relations for viscous stresses and heat fluxes in the order of the Knudsen number. For fluid flows with small Knudsen number \((Kn \to 0)\), the leading order terms dominate and the Navier-Stokes equations are obtained by truncating the higher order terms. For fluid flows with high Knudsen numbers, the leading order approximation of the constitutive relations that appear in the Navier-Stokes equations is not valid. The Burnett equations used in this study are obtained by keeping the second-order terms in the constitutive relations for the viscous stresses and the heat transfer rates (Chapman and Cowling 1970; Wang Chang, C.S. and Uhlenbeck 1970). The conventional Burnett equations and augmented Burnett equations have been described in Chapter 4.

The second-order truncation is appropriate for MEMS flows with the Knudsen number in the order of 0.1 and the resulting Burnett equations should provide an accurate model for microflows in the continuum-transition regime. The numerical methods developed for solving the Navier-Stokes equations in CFD can be readily adopted for the Burnett equations (Guo et al. 1999; Agarwal et al. 1999; Balakrishnan and Agarwal 1996; Zhong et al. 1991). As a result, the computational resources needed for solving the Burnett equations can be orders of magnitude less than that for

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In this Chapter, a validated numerical algorithm developed for the Navier-Stokes equations is applied to solve the conventional Burnett equations. The Burnett equations have been used to calculate hypersonic flows with low density (Guo et al. 1999; Agarwal et al. 1999; Balakrishnan and Agarwal 1996; Zhong et al. 1991). The flow speeds in microdevices are generally low. Most, if not all, CFD schemes developed for high-speed flows are not effective for flows at low speed. An all-Mach-number formulation as implemented in a Navier-Stokes solver, ALLSPD3D (Shuen et al. 1993), is applied in this study. The formulation is described in the following sections. As the all-Mach-number algorithm provides a strong coupling between the momentum and the energy at low speeds, the resulting Burnett equations solver can be a fairly accurate numerical tool for studying the flow and the heat transfer properties of microflows.

The new solver is validated using flows through microchannels. Results are compared with those obtained by using the Navier-Stokes equations with and without slip-wall conditions. For the cases considered, with the reference Knudsen number as large as 0.02, there is good agreement between the Navier-Stokes solutions and the Burnett solutions when the same type of wall boundary conditions is applied. The effects of Knudsen number on the flow and the heat transfer characteristics of the microchannel are also discussed.

Governing Burnett Equations

The three-dimensional unsteady conventional Burnett equations are equations
(4.24-26) combined with the constitutive equation (4.53). Equations (4.24-26) are the conservation equations of the Boltzmann equation for mass, momentum and translational energy, respectively. Equation (4.53) is the constitutive relation for the nonlinear second order viscous stress and heat flux, which can be obtained from the Chapman-Enskog expansion theory. Removing the time-derivative terms in equations (4.24-26), the three-dimensional steady conventional Burnett equations written in a generalized nonorthogonal coordinate system can be expressed in a strong conservation form as

\[
\frac{\partial}{\partial \xi} (\tilde{E} - \tilde{E}_v^{(1)} - \tilde{E}_v^{(2)}) + \frac{\partial}{\partial \eta} (\tilde{F} - \tilde{F}_v^{(1)} - \tilde{F}_v^{(2)}) + \frac{\partial}{\partial \zeta} (\tilde{G} - \tilde{G}_v^{(1)} - \tilde{G}_v^{(2)}) = 0
\]

(9.1)

where the vectors, \(\tilde{E}, \tilde{F}, \tilde{G}, \tilde{E}_v^{(1)}, \tilde{F}_v^{(1)}, \tilde{G}_v^{(1)}, \tilde{E}_v^{(2)}, \tilde{F}_v^{(2)},\) and \(\tilde{G}_v^{(2)},\) are defined as

\[
\tilde{E} = (\xi_x E + \xi_y F + \xi_z G)/J
\]

(9.2)

\[
\tilde{F} = (\eta_x E + \eta_y F + \eta_z G)/J
\]

(9.3)

\[
\tilde{G} = (\zeta_x E + \zeta_y F + \zeta_z G)/J
\]

(9.4)

\[
\tilde{E}_v^{(1)} = (\xi_x E_v^{(1)} + \xi_y F_v^{(1)} + \xi_z G_v^{(1)})/J
\]

(9.5)

\[
\tilde{F}_v^{(1)} = (\eta_x E_v^{(1)} + \eta_y F_v^{(1)} + \eta_z G_v^{(1)})/J
\]

(9.6)

\[
\tilde{G}_v^{(1)} = (\zeta_x E_v^{(1)} + \zeta_y F_v^{(1)} + \zeta_z G_v^{(1)})/J
\]

(9.7)

\[
\tilde{E}_v^{(2)} = (\xi_x E_v^{(2)} + \xi_y F_v^{(2)} + \xi_z G_v^{(2)})/J
\]

(9.8)

\[
\tilde{F}_v^{(2)} = (\eta_x E_v^{(2)} + \eta_y F_v^{(2)} + \eta_z G_v^{(2)})/J
\]

(9.9)

\[
\tilde{G}_v^{(2)} = (\zeta_x E_v^{(2)} + \zeta_y F_v^{(2)} + \zeta_z G_v^{(2)})/J
\]

(9.10)
In the above expressions, $\xi$, $\eta$, and $\zeta$ denote the generalized spatial coordinates, and $x$, $y$, and $z$ are the physical Cartesian coordinates. $J$ represents the transformation Jacobian from the physical Cartesian coordinates to the generalized spatial coordinates. The coordinate transformation relations for derivatives and metrics are given in Appendix B. $E$, $F$, and $G$ are the convection flux vectors, defined as

\[
E = \begin{bmatrix}
\rho u \\
\rho u^2 + p \\
\rho uv \\
\rho uw \\
(pE_z + p)u
\end{bmatrix}
\]  
(9.11)

\[
F = \begin{bmatrix}
\rho v \\
\rho uv \\
\rho v^2 + p \\
\rho vw \\
(pE_z + p)v
\end{bmatrix}
\]  
(9.12)

\[
G = \begin{bmatrix}
\rho w \\
\rho uw \\
\rho vw \\
\rho w^2 + p \\
(pE_z + p)w
\end{bmatrix}
\]  
(9.13)

$E^{(1)}$, $F^{(1)}$, and $G^{(1)}$ are the first-order (Navier-Stokes-order) viscous flux vectors, defined as

\[
E^{(1)} = \begin{bmatrix}
0 \\
\tau^{(1)}_{xx} \\
\tau^{(1)}_{xy} \\
\phi^{(1)}_x
\end{bmatrix},
F^{(1)} = \begin{bmatrix}
0 \\
\tau^{(1)}_{xy} \\
\tau^{(1)}_{yy} \\
\phi^{(1)}_y
\end{bmatrix},
G^{(1)} = \begin{bmatrix}
0 \\
\tau^{(1)}_{xz} \\
\tau^{(1)}_{yz} \\
\phi^{(1)}_z
\end{bmatrix}
\]  
(9.14)
\( \Phi^{(i)} = u \tau_{ix}^{(i)} + v \tau_{iy}^{(i)} + w \tau_{iz}^{(i)} + q_x^{(i)} \)
\( \Phi_y^{(i)} = u \tau_{yx}^{(i)} + v \tau_{yy}^{(i)} + w \tau_{yz}^{(i)} + q_y^{(i)} \)
\( \Phi_z^{(i)} = u \tau_{zx}^{(i)} + v \tau_{zy}^{(i)} + w \tau_{zz}^{(i)} + q_z^{(i)} \)

\[ \text{E}_v^{(2)}, \text{F}_v^{(2)}, \text{and} \ G_v^{(2)} \text{ are the second-order (Burnett-order) viscous flux vectors, defined as,} \]

\[ \text{E}_v^{(2)} = \begin{bmatrix} 0 \\ \tau_{xx}^{(2)} \\ \tau_{xy}^{(2)} \\ \tau_{xz}^{(2)} \\ \phi_x^{(2)} \end{bmatrix}, \quad \text{F}_v^{(2)} = \begin{bmatrix} 0 \\ \tau_{yx}^{(2)} \\ \tau_{yy}^{(2)} \\ \tau_{yz}^{(2)} \\ \phi_y^{(2)} \end{bmatrix}, \quad \text{G}_v^{(2)} = \begin{bmatrix} 0 \\ \tau_{zx}^{(2)} \\ \tau_{zy}^{(2)} \\ \tau_{zz}^{(2)} \\ \phi_z^{(2)} \end{bmatrix} \]

\[ \phi_x^{(2)} = u \tau_{xx}^{(2)} + v \tau_{xy}^{(2)} + w \tau_{xz}^{(2)} + q_x^{(2)} \]
\[ \phi_y^{(2)} = u \tau_{yx}^{(2)} + v \tau_{yy}^{(2)} + w \tau_{yz}^{(2)} + q_y^{(2)} \]
\[ \phi_z^{(2)} = u \tau_{zx}^{(2)} + v \tau_{zy}^{(2)} + w \tau_{zz}^{(2)} + q_z^{(2)} \]

where \( \rho, p, u, v, \) and \( w \) are the density, pressure, and Cartesian velocity components, respectively. The total energy is defined as

\[ E_t = e + \frac{(u^2 + v^2 + w^2)}{2} \]

with \( e \) being the thermodynamic internal energy. In equations (9.14-17), the first-order viscous stress and heat flux, \( \tau^{(i)}_{ij} \) and \( q^{(i)}_j \), and the corresponding second-order expressions, \( \tau^{(2)}_{ij} \) and \( q^{(2)}_j \), are presented in the Chapter 4.

**Numerical Methods**

In most MEMS devices, the microflows are characterized with high Knudsen number and low Mach number. As the value of the Knudsen number in a microflow is typically higher than 0.01, the rarefied gas effect is important. This is reason that the
compressible form of the Burnett equations is used in this work. Most of the computational methods developed for the compressible Navier-Stokes equations are ineffective for low-Mach-number flows. This is due to the round-off error caused by the singular pressure gradient term in the momentum equations and the stiffness caused by the wide disparities in eigenvalues. To circumvent these two problems in the current study of the microflow and heat transfer, an all-Mach-number formulation (Chen et al. 1995) is adopted. The ALLSPD3D code solves the three-dimensional Navier-Stokes equations using central differencing with artificial dissipation.

All-Mach-Number Formulation

In the all-Mach-number formulation, the system’s eigenvalues are rescaled and the pressure variable is decomposed into a constant reference pressure $p_0$ and a gauge pressure $p_s$. The resulting Burnett equations can be written as

$$
\Gamma \frac{\partial}{\partial \tau^*} \hat{Q} + \frac{\partial}{\partial \xi} (\hat{E}_\nu - \hat{E}_\nu^{(1)} - \hat{E}_\nu^{(2)}) + \frac{\partial}{\partial \eta} (\hat{F}_\nu - \hat{F}_\nu^{(1)} - \hat{F}_\nu^{(2)}) + \frac{\partial}{\partial \zeta} (\hat{G}_\nu - \hat{G}_\nu^{(1)} - \hat{G}_\nu^{(2)}) = 0 \quad (9.19)
$$

where the primitive variable vector $\hat{Q}$ and the time preconditioning matrix $\Gamma$ are given as

$$
\hat{Q} = (p_s, u, v, w, h)^T / J \\
\Gamma = \left( \begin{array}{cccc}
1 / \beta & 0 & 0 & 0 \\
1 / \beta & \rho & 0 & 0 \\
v / \beta & 0 & \rho & 0 \\
w / \beta & 0 & 0 & \rho \\
H / \beta - 1 & \rho u & \rho v & \rho w & \rho
\end{array} \right) \quad (9.21)
$$

$\tau^*$ is a pseudo-time and $\beta$ is a parameter for rescaling the eigenvalues of the new
system of equations. $h = e + \rho \, u$ is the specific enthalpy and $H$ the total specific enthalpy. The eigenvalues (in the $\xi$-direction) in pseudo-time can be obtained from the matrix $\Gamma^{-1}A$, where $A$ is the Jacobian $\partial \tilde{E}/\partial \tilde{Q}$. The eigenvalues for a real gas are

$$\lambda = \left( \frac{U_1 U_2 U_3}{2} \left[ U_4 (1 + \frac{\beta}{a^2}) \pm \sqrt{U_4^2 (1 - \frac{\beta}{a^2}) + 4 \beta (\alpha_1^2 + \alpha_2^2 + \alpha_3^2)} \right] \right)$$

(9.22)

where $a$ is the speed of sound, $\alpha_1 = \xi_x$, $\alpha_2 = \xi_y$, $\alpha_3 = \xi_z$, and $U$ is the contravariant velocity component defined as $U = \alpha_1 u + \alpha_2 v + \alpha_3 w$. To obtain well-conditioned eigenvalues, the scaling factor $\beta$ is taken to be $\beta = u^2 + v^2 + w^2$ such that all the eigenvalues will have the same order of magnitude.

Equation (9.19) is the form of the conventional Burnett equations to be solved numerically. Since only steady-state problems are of interest in the present study, numerical solutions of equation (9.19) are obtained when the numerical iteration from an initial condition in pseudo-time has converged.

LU-SGS Scheme

In the linearization of equation (9.19), the convective terms and the Navier-Stokes-order terms of viscous stress and heat flux are treated implicitly. The Burnett order terms are treated explicitly. After the linearization and applying a first-order forward finite differencing in time, equation (9.19) can be expressed in the following form,
\[
\begin{align*}
\Gamma + \Delta \tau^\ast \left( \frac{\partial A}{\partial \xi} - \frac{\partial \mathbf{R}_{\xi \xi}}{\partial \xi} \right) + \Delta \tau^\ast \left( \frac{\partial \mathbf{B}}{\partial \eta} - \frac{\partial \mathbf{R}_{\eta \eta}}{\partial \eta} \right) \\
+ \Delta \tau^\ast \left( \frac{\partial \mathbf{C}}{\partial \xi} - \frac{\partial \mathbf{R}_{\xi \xi}}{\partial \xi} \right) \Delta \mathbf{Q} = -\Delta \tau^\ast \text{RHS}^p
\end{align*}
\] (9.23)

where

\[
\text{RHS}^p = \left[ \frac{\partial (\mathbf{E} - \mathbf{E}^{(1)})^p}{\partial \xi} + \frac{\partial (\mathbf{F} - \mathbf{F}^{(1)})^p}{\partial \eta} + \frac{\partial (\mathbf{G} - \mathbf{G}^{(1)})^p}{\partial \zeta} \right]
- \left[ \frac{\partial (\mathbf{E}^{(1)})^p}{\partial \xi} + \frac{\partial (\mathbf{F}^{(1)})^p}{\partial \eta} + \frac{\partial (\mathbf{G}^{(1)})^p}{\partial \zeta} \right] + \mathbf{D}_e
\] (9.24)

where the superscript \( p \) denotes a counter for the numerical iteration. The second term in RHS is the Burnett order one. \( \mathbf{A}, \mathbf{B}, \) and \( \mathbf{C} \) are the convective term Jacobians of \( \mathbf{A} = \partial \mathbf{E} / \partial \mathbf{Q}, \mathbf{B} = \partial \mathbf{F} / \partial \mathbf{Q} \) and \( \mathbf{C} = \partial \mathbf{G} / \partial \mathbf{Q} \). \( \mathbf{R}_{\xi \xi}, \mathbf{R}_{\eta \eta}, \) and \( \mathbf{R}_{\zeta \zeta} \) are the viscous Jacobians of the Navier-Stokes order terms, \( \mathbf{R}_{\xi \xi} = \partial \mathbf{E}^{(1)} / \partial \mathbf{Q}, \mathbf{R}_{\eta \eta} = \partial \mathbf{F}^{(1)} / \partial \mathbf{Q} \) and \( \mathbf{R}_{\zeta \zeta} = \partial \mathbf{G}^{(1)} / \partial \mathbf{Q} \), and \( \mathbf{Q}^{p+1} = \mathbf{Q}^p + \Delta \mathbf{Q} \). The expressions for these Jacobians have been finished in Shuen et al. (1993) and also are given in Appendix B for completeness. \( \mathbf{D}_e \) contains the explicit second and forth viscous dissipation terms that will be defined later.

The lower-upper symmetric Gauss-Seidel (LU-SGS) scheme described here was originally developed for Euler and Navier-Stokes calculations without preconditioning (Yoon and Jameson 1987; Yoon et al. 1989). With the current time preconditioning, the LU-SGS scheme has to be modified to incorporate the preconditioning matrix \( \Gamma \). The LHS convection terms in equation (9.23) need to be modified to include the preconditioning matrix. For example, in the \( \xi \)-direction,
where $\hat{A} = \Gamma^{-1} A$. $\hat{A}$ is then split into two parts,

$$
\hat{A} = \frac{1}{2} (\hat{A} + \alpha \lambda_{\text{max}} I) + \frac{1}{2} (\hat{A} - \alpha \lambda_{\text{max}} I) = \hat{A}^+ + \hat{A}^-
$$

where $\lambda_{\text{max}}$ is the absolute value of the maximum eigenvalues in the $\xi$-direction at each grid point, $\alpha$ is a parameter greater than 1, and $I$ is the unit matrix. The term $\partial A / \partial \xi$ in equation (9.23) is then approximated by the following one-sided operator,

$$
\frac{\partial A}{\partial \xi} = \frac{\partial^-}{\partial \xi} (\Gamma \hat{A}^+) + \frac{\partial^+}{\partial \xi} (\Gamma \hat{A}^-) \tag{9.26}
$$

where

$$
\Gamma \hat{A}^+ = \frac{1}{2} \Gamma (\hat{A} + \alpha \lambda_{\text{max}} I) - \frac{1}{2} (\hat{A} + \alpha \lambda_{\text{max}} I)
$$

The operator $\partial^- / \partial \xi$ and $\partial^+ / \partial \xi$ in equation (9.26) are the first order backward and forward differencing operators, respectively. The same procedures are also applied to $\partial B / \partial \eta$ and $\partial C / \partial \zeta$. It is seen that the effect of the above eigenvalues augmentation is equivalent to adding a second-order central-differencing dissipation term (scaled by the local maximum eigenvalues) to the implicit operator. Therefore, the discretized governing equations for LU-SGS scheme can be written as follows,

$$
\begin{align*}
\Gamma + \Delta \tau^+ \left( \frac{\partial A}{\partial \xi} - \frac{\partial R}{\partial \xi} \right) + \Delta \tau^- \left( \frac{\partial B}{\partial \eta} - \frac{\partial R}{\partial \eta} \right) + \Delta \tau^+ \left( \frac{\partial C}{\partial \zeta} - \frac{\partial R}{\partial \zeta} \right) + \Delta \tau^- \left( \frac{\partial D}{\partial \zeta} \right) + \Delta \tau^+ D_2 \right] = \Delta \tau^- \text{RHS}^p
\end{align*}
$$

where the second order dissipation term for the implicit operator of the LHS is
the explicit dissipation terms, including the forth and second order, are

$$D_{ex} = \frac{vis_4}{24} \Gamma \left[ \lambda_{\text{max}} \frac{\partial^4}{\partial \xi^4} \hat{Q} + \lambda_{\text{max}} \frac{\partial^4}{\partial \eta^4} \hat{Q} + \lambda_{\text{max}} \frac{\partial^4}{\partial \zeta^4} \hat{Q} \right]$$

$$+ \frac{vis_2}{6} \Gamma \left[ \lambda_{\text{max}} \frac{\partial^2}{\partial \xi^2} \hat{Q} + \lambda_{\text{max}} \frac{\partial^2}{\partial \eta^2} \hat{Q} + \lambda_{\text{max}} \frac{\partial^2}{\partial \zeta^2} \hat{Q} \right]$$

(9.29)

where $|\lambda_{\text{max}}, \lambda_{\text{max}}|$ and $|\lambda_{\text{max}}|$ are the absolute values of the maximum eigenvalues in the $\xi, \eta$ and $\zeta$ directions. The parameters $vis_4$ and $vis_2$ are used to define the dissipation strength.

During the discretization, the Second-order accurate central differencing is used to discretize the spatial derivative terms in equation (9.27) for both the explicit and the implicit operators.

The LU-SGS scheme utilizes the following factorization procedure to obtain the solution,

$$MAQ = b$$

(9.30)

$$(L + D)D^{-1}(U + D)\Delta \hat{Q} = b$$

(9.31)

Equations (9.31) can be solved in the following steps,

Step 1 $$(L + D)\Delta \hat{Q} = b$$

Step 2 $$(U + D)\Delta \hat{Q} = D(\Delta \hat{Q}^*)$$

(9.32)

Step 3 $\hat{Q}^{new} = \hat{Q}^* + \Delta \hat{Q}$$

Where $M$ and $b$ are the LHS and RHS of equation (9.27), respectively. The $L$, $U$
and D are the non-zero, off-diagonal lower, upper and diagonal part of matrix M, respectively.

Pseudo-Time Step

In equation (9.23), \( \Delta \tau^* \) is the pseudo-time which is determined from the eigenvalue analysis. Using the previously defined pseudo-time eigenvalues of equation (9.22), the maximum eigenvalues in each direction are

\[
\lambda_A = \frac{1}{2} \left[ U_A (1 + \frac{\hat{\beta}}{a^2}) + \sqrt{U_A^2 (1 - \frac{\hat{\beta}}{a^2}) + 4\hat{\beta}(\xi_x^2 + \xi_y^2 + \xi_z^2)} \right]
\]

\[
\lambda_B = \frac{1}{2} \left[ U_B (1 + \frac{\hat{\beta}}{a^2}) + \sqrt{U_B^2 (1 - \frac{\hat{\beta}}{a^2}) + 4\hat{\beta}(\eta_x^2 + \eta_y^2 + \eta_z^2)} \right]
\]

\[
\lambda_C = \frac{1}{2} \left[ U_C (1 + \frac{\hat{\beta}}{a^2}) + \sqrt{U_C^2 (1 - \frac{\hat{\beta}}{a^2}) + 4\hat{\beta}(\zeta_x^2 + \zeta_y^2 + \zeta_z^2)} \right]
\]

where the contravariant velocity components are

\[
U_A = \xi_x u + \xi_y v + \xi_z w
\]

\[
U_B = \eta_x u + \eta_y v + \eta_z w
\]

\[
U_C = \zeta_x u + \zeta_y v + \zeta_z w
\]

and the scaling factor \( \hat{\beta} = u^2 + v^2 + w^2 \) is modified according to

\[
\hat{\beta} = \min\{a^2, \max(\beta, U_{\text{ref}}^2)\}
\]

where \( U_{\text{ref}} \) is the reference velocity determined by the upstream velocity

\[
U_{\text{ref}}^2 = u_{\text{ref}}^2 + v_{\text{ref}}^2 + w_{\text{ref}}^2.
\]

The pseudo-time, \( \Delta \tau^* \), is then calculated by the following
equation,

\[ \Delta \tau' = CFL/(\lambda_\lambda^2 + \lambda_B^2 + \lambda_r^2)^{1/2} \]  

(9.35)

where \( CTL \) is the CFL number.

Wall Boundary Conditions

It is generally recognized that no velocity-slip/no temperature-jump (VSTJ) boundary conditions should be applied on a wall when solving the Navier-Stokes equations for \( Kn<0.001 \). In the slip-flow (0.001<\( Kn<0.1 \)) and the continuum transition (0.1<\( Kn<10 \)) regimes, the VSTJ conditions should be used for both the Navier-Stokes equations and the Burnett equations. The VSTJ conditions can be obtained by an approximate analysis of the motion of a monatomic gas near an isothermal wall. The uncoupled VSTJ boundary conditions used here are obtained by simplifying the Maxwell-Smoluchowski formulae of equations (4.70) and (4.71),

\[ u_s-u_w = \frac{2-a_v}{a_v} \lambda \left( \frac{\partial u}{\partial y} \right), \]  

(9.36)

\[ T_s-T_w = \frac{2-a_v}{a_v} \frac{2\gamma}{\gamma+1} \frac{\lambda}{Pr} \left( \frac{\partial T}{\partial y} \right), \]  

(9.37)

\( \lambda \) denotes the mean free path of gas, and \( Pr \) the Prandtl number. Care should be exercised in the numerical implementation of equations (9.36) and (9.37) due to the mixed-type boundary conditions. An explicit form of equations (9.36) and (9.37) at pseudo-time level \( (p+1) \) is used,

\[ u_{s}^{p+1} - u_w = \left[ \frac{2-a_v}{a_v} \lambda \left( \frac{\partial u}{\partial y} \right) \right]^p \]  

(9.38)
Together with the pressure condition on the wall, equations (9.27), (9.36) and (9.37) form a system of equations that is solved numerically by using the modified LU-SGS method.

Numerical Results and Discussions

The Burnett equations solver has been applied to flows in two-dimensional microchannels, as shown in Figure 91. The inflow velocities, \( u_{in} \) and \( v_{in} \), and temperature \( T_{in} \) are given as the inflow condition. At the downstream boundary, the outlet pressure \( p_{out} \) is assigned. The isothermal wall temperature is \( T_w \). The operating conditions are:

\[
\begin{align*}
    u_{in} & = 133 \text{ m/s} \\
    v_{in} & = 0 \\
    T_{in} & \quad \text{isothermal}
\end{align*}
\]

**Microchannel Flow**

![Microchannel Flow Diagram](image)

Figure 91. Simulated micro-geometry.
The velocity profiles at \( \frac{x}{h} = 2.5 \) are shown in Figure 92. The solutions obtained by using both the Navier-Stokes equations and the conventional Burnett equations are included. In one set, the wall velocity-slip/temperature-jump conditions (Slip) are used while other set uses the No-slip conditions. The value of the Knudsen number is 0.01, which is evaluated at the exit of the channel. The flow Reynolds number is about 66. The grid size is 121\( \times \)50. A comparison of the streamwise velocity profiles obtained by using the Burnett equations shows that, with the VSTJ conditions, the flow is slightly slower than that without it at the center region of the channel. The difference between the two solutions becomes indistinguishable away from this center region. For the solutions obtained by using the Navier-Stokes equations, the comparison appears very similar to that for the Burnett equations. In fact, the solutions obtained by using the Navier-Stokes and the Burnett equations nearly overlap one another when the same type of condition is used on the wall, i.e. Slip vs. No-slip. This agreement between the two solutions appears reasonable considering the small value of the Knudsen number. The results suggest that the second-order viscous stress terms have insignificant contribution to the momentum.

\[ T_{in} = 300 \text{K} \]

\[ T_{w} = 300 \text{K} \]

The gas constants used are,

\[ \gamma = 1.4 \]

\[ \text{Pr} = 0.72 \]

\[ R = 287.04 \text{m}^2 / (\text{s}^2 \text{K}) \]
transfer in this microfluid flow.

Figure 92. Comparison of velocity profiles at $x/h=2.5$, $Re=66$.

Figure 93 shows a streamwise velocity profile comparison for a case with $Kn=0.02$. The mean free path is increased by a factor of two from the previous case by reducing the exit pressure by one-half. The value of the Reynolds number is 33. In order to achieve converged solutions, the grid number across the channel in the direction normal to the wall is reduced. The grid size is $121 \times 30$. The magnitudes of the velocity at the centerline are slightly higher than that of the case with $Kn=0.01$. Again, there is no significant difference between the solutions obtained by the Burnett equations and the Navier-Stokes equations when the same type of wall boundary conditions is used. Figures 94 and 95 show the comparison of the temperature distributions for these two cases. The calculated values of the temperature at the
centerline are lower for cases with $Kn=0.02$ than with 0.01 by about 4K. For $Kn=0.01$, the difference among the numerical solutions is contributed mainly by the different boundary conditions. For the cases with $Kn=0.02$, there is a slight variation between the solutions obtained by using the Burnett and the Navier-Stokes equations, even when the same type of boundary conditions is used. The observations seem to suggest, as it should be, that flows calculated by using the Burnett equations can progressively diverge away from those obtained by using the Navier-Stokes equation as the value of $Kn$ increases. A further reduction of the grid number in the wall-normal direction is found necessary to obtain solutions for cases with high value of $Kn$. This may be due to the known instability of the conventional Burnett equations to disturbances with small wavelength (Agarwal et al. 1999; Balakrishnan and Agarwal 1996; Zhong et al. 1991). Other forms of the Burnett equations have been proposed and shown to produce stable solutions for hypersonic applications. It should also be noted that the VSTJ conditions (Schaaf and Chambre 1961) are approximated series expansions located one mean-free-path away from the wall. Numerical instability, therefore, can occur in the wall region when the local computational grid sizes are significantly smaller than the local mean free path. A modification of the series expansion can be effective in reducing the numerical instability, which is an effort beyond the scope of this work.
Figure 93. Comparison of velocity profiles at $x/h=2.5$. Re=33.

Figure 94. Comparison of temperature distributions at $x/h=2.5$. Re=66
Figure 95. Comparison of temperature distributions at $x/h=2.5$. $Re=33$.

The streamwise velocity profiles at five different streamwise locations are shown in Figures 96 and 97 for $Kn=0.01$ and $Kn=0.02$, respectively. The solutions obtained by using the No-slip conditions are also included for comparison. The top-hat velocity distribution used at the inlets of both cases gradually develops into parabolic-like profiles at the later part of the channel. The case with $Kn=0.02$ also appears to have a progressively higher velocity than that with $Kn=0.01$. Overall, the calculated flow speed with VSTJ is slightly smaller than without VSTJ.

The inlet temperatures for both cases are set at 300 K, which is the same as the wall temperature. The computed temperature profiles at four streamwise locations are shown in Figures 98 and 99 for $Kn=0.01$ and 0.02, respectively. The temperature decreases as the flow develops downstream, with a more significant change for the high Knudsen case.
Figure 96. Velocity profiles. Re=66.

Figure 97. Velocity profiles. Re=33

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Figure 98. Temperature profiles. Re=66.

Figure 99. Temperature profiles. Re=33.
Figure 100 compares the wall-slip velocities obtained by using the Burnett and the Navier-Stokes equations for the low and high Knudsen cases. For the same Knudsen number, there is little difference between the Burnett and the Navier-Stokes solutions. The wall-slip velocity for the case with $Kn=0.02$ is higher than that for the $Kn=0.01$ case and, at the exit, the slip-velocity for the high $Kn$ case is nearly three times higher than that for the low $Kn$ case.

![Graph showing gas velocity slip on the wall](image)

Figure 100. Gas velocity slip on the wall.

Figure 101 shows the distributions of the gas temperature adjacent to the wall for the two cases. No significant difference is observed between the Navier-Stokes and the Burnett solutions. The gas temperature is initially close to the wall temperature and remains so for the entire microchannel for the case with $Kn=0.01$. For the $Kn=0.02$ case, the gas temperature on the channel wall continues to drop to about 3 K lower than the wall temperature at the exit.
Figure 101. Comparison of gas temperature on the wall.

Figure 102 shows the wall pressure distributions. For both the low and high Knudsen number cases, the VSTJ conditions have a significant influence on the wall pressure variations. Except for a region of initial transition from uniform inlet conditions, the wall pressure varies in nearly a linear fashion. The values are lower when the VSTJ conditions are used.
Figure 102. Wall pressure distributions.

Figure 103 shows the streamwise variation of the heat transfer coefficients for the two cases. Immediately downstream of the inlet, the solutions obtained without imposing the VSTJ conditions are negative, indicating a heat transfer to the wall. In the same region, the solutions obtained with the VSTJ conditions did not become negative. Beyond the initial transition region, the heat transfer coefficients are positive for $Kn=0.01$, regardless of the imposition of the VSTJ conditions. For the high Knudsen number case, however, the heat transfer to the microfluid flows is significantly higher compared with the low Knudsen case. Recall that Figures 98 and 99 show that the temperature for the high Knudsen case is, in general, lower than that for the low Knudsen number case. This is a trend that has also been observed in the DSMC solutions of similar low-speed microchannel flows with a wider range of Knudsen numbers ($<0.8$) (Fang and Liou 2001).
Figure 103. Heat transfer coefficient distributions on the wall.

Concluding Remarks

The conventional Burnett equations are applied to two-dimensional microchannel flows with $Kn$ up to 0.02. A numerical method to solve the three-dimensional Burnett equations is developed. Based on the implicit method used in ALLSPD, this method solves the first-order terms of viscous stress and heat flux implicitly and the higher-order terms explicitly using central differencing. The new Burnett solver is validated using flows through microchannels. For the range of Knudsen number used in this study, the difference between the solutions obtained by using the Burnett and the Navier-Stokes equations is minimal when the same type of wall boundary conditions is used. As expected, the wall slip-velocity and temperature-jump increase with elevated value of the Knudsen numbers. The results show that the
heat transfer to the microfluid flow also increases with the Knudsen number despite the low temperature in the bulk of the flow, a phenomenon that has also been observed in DSMC simulations of low-speed microchannel flow with a broader range of Knudsen number. Modification to the VSTJ conditions may be needed for the calculations of high Knudsen number microchannel flows.
CHAPTER X

SUMMARY AND CONCLUSIONS

Summary

The primary objective of this dissertation is to simulate numerically and study the heat transfer and flow characteristics in fluidic MEMS. In the microfluidic MEMS applications, the gas mean-free-path is comparable to the characteristic length scale; that is, the Knudsen number could be large. The traditional mathematical models of continuum flows are based on the Navier-Stokes equations, and these equations become invalid for high Knudsen number applications because of their linear constitutive relations for viscous stress and heat flux.

The Boltzmann equation was briefly derived with the assumptions of a dilute gas and molecular chaos, which is the governing equation to describe gas microflows. The DSMC methodology and its basic kinetic theories were introduced. It has been shown that the Boltzmann equation can be derived from the DSMC procedures, indicating that DSMC is a particle method that can be as accurate as the Boltzmann equation. Also, the Burnett general conservative equations were also derived in detail from the Boltzmann equation. The derivation of the high-order constitutive relations for dilute gases from the Boltzmann equation and the Chapman-Enskog expansion was presented, along with the detailed expressions for the conventional Burnett equations and the augmented Burnett equations.

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The first application investigated was supersonic microchannel flows with the DSMC method. The effects of $Kn$ on the heat transfer and flow characteristics were studied for three different values of $Kn$. For the application of low-speed flows, the inlet/outlet DSMC boundary conditions that have been successfully applied to hypersonic rarefied gas flows are not valid. A modified DSMC method with implicit boundary has been developed for subsonic flows. The local mean velocity, temperature and number density near the boundaries are used to determine the number of molecules entering the computation domain and their corresponding velocity components and internal energy. The pressure exit condition is physically imposed. Furthermore, the method enforces mass conservation and is consistent with the characteristic theory of subsonic flows. This implicit algorithm was applied to micro-Couette flows and micro-Poiseuille flows for values of $Kn$ ranging between 0.06 and 0.72. Where appropriate, the calculated velocity profile, velocity slip, temperature profile, and temperature jump were compared with analytical solutions derived from the Navier-Stokes equations using the first-order and second-order slip boundary conditions. The thermodynamics of the computed flows with the effects of $Kn$ were also examined.

With the development of affordable HPCC, a Beowulf system of PC cluster, CEPCOM, was set up in 2001 in the Computational Fluid Dynamics laboratory. The new DSMC algorithm was parallelized using MPI. The parallel efficiency was benchmarked on CEPCOM for simulations of a micro-Poiseuille flow. The speedup can be at least 15 on 32 processors. The parallel DSMC algorithm was also applied to
flows in a patterned microchannel with surface heating. A dedicated parallel, unsteady
DSMC algorithm was developed to study the time-dependent behavior of an initially
chaotic micro-Couette flow, and both two-dimensional and three-dimensional
geometries were studied. An applied artificial forcing was used to drive the flow into
forming organized patterns in a microchannel with size of 800×60×320 gas mean-
free-path. The organized flow patterns appear similar to that observed in Taylor-
Gortler problems. Vortical structures have also been identified that are associated
with a hierarchy of waves, consisting of a fundamental mode and its harmonics.

The conventional Burnett equations were applied to a two-dimensional
microchannel flows with $Kn$ up to 0.02. A numerical method for solving the three-
dimensional Burnett equations was developed. This method solves the first-order
terms of viscous stress and heat flux implicitly and the higher-order terms explicitly,
by using central differencing. For the range of Knudsen number used in this study, the
solutions obtained by using the conventional Burnett and the Navier-Stokes equations
were compared when the same type of wall boundary conditions were imposed.

Conclusions

DSMC and Burnett equations are accurate methods to simulate and study the
heat transfer and the flow characteristics of microflows in fluidic MEMS from
molecular and continuum point of view, respectively.

The proposed implicit treatment of subsonic flow boundaries is robust and
appropriate for DSMC simulation MEMS flows. The method enforces mass
conservation and is consistent with the characteristic theory of subsonic flows. The
simulation results show that the mass influx due to thermal fluctuations represents a significant portion of the overall mass flux balance in subsonic MEMS flows.

In the micro-Couette flows, the DSMC results indicate that the velocity profile exhibits a nonlinear wavy behavior that has not been reported previously. The velocity slip and temperature jump on the wall and the temperature profile agree well with the analytical solutions obtained from the Navier-Stokes equations using the first-order slip boundary condition.

Comparisons of the velocity profiles and velocity slips in the micro-Poiseuille flows show that the DSMC solutions agree well with the analytical solutions derived from the Navier-Stokes equations using both the first-order and second-order slip boundary conditions for the low $Kn$ cases ($Kn < 0.2$). For the high $Kn$ case ($Kn > 0.2$), there is a better agreement with the analytical solutions using the second-order slip boundary conditions. It might be concluded that the higher-order slip boundary conditions should be used to mathematically model high Knudsen number microflows.

In the DSMC simulations, the heat transfer characteristics of microchannel flows can vary significantly with Knudsen number. For the two-dimensional supersonic flows in this study, there is a significant increase of wall heat transfer with increasing Knudsen number, and the enhanced wall heat transfer is mainly caused by the increased number rate of molecules that impact the wall. In the calculated two-dimensional subsonic microfluid flows, the wall heat transfer decreases with increasing Knudsen number. As the value of the Knudsen number for a typical

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MEMS device can be quite high, this unique behavior of the wall heat transfer might have a significant bearing on the development and the design of MEMS.

The DSMC algorithm can be parallelized efficiently for cluster computers, such as the CEPCOM. The necessary communication time does not dominate over the calculation time in parallel DSMC (PDSMC) simulations, and there is not much calculation overhead for the parallelization. The parallel DSMC algorithm can provide significant reductions in the total computing time and the memory storage required in each computing node. The PDSMC also make it practical to simulate more realistic and complicated problems with DSMC, such as the forced chaotic flows studied in this dissertation.

In the forced chaotic flow studies, an applied artificial forcing was used to drive the flow into organized patterns, similar to that observed in Taylor-Gortler problems. Vortical structures have also been identified that are associated with a hierarchy of waves, consisting of a fundamental mode and its harmonics. Despite the fact that the forcing amplitude may be unrealistic, the results of the simulations show that the particle-based DSMC method has the capability to capture the nonlinear evolution of harmonic waves, which is generally recognized as a necessary route that precedes laminar breakdown. This finding, we believe, has not been reported in the open literature. The results for the limited window of parameters presented in this work suggest that DSMC can capture important flow phenomena at microscales.

The new Burnett equation solver is validated for the case of microchannel flows. For the range of Knudsen number studied in this dissertation, the difference
between the solutions obtained by using the Burnett and the Navier-Stokes equations is minimal when the same type of wall boundary conditions is used. The wall slip-velocity and temperature-jump increase with elevated Knudsen number values. The results show that the heat transfer to the microfluid flow also varies significantly with the Knudsen number despite the low temperature in the bulk of the flow, a phenomenon that has also been observed in DSMC simulations of low-speed microchannel flow with a broader range of Knudsen number.

Future

This dissertation research forms a base for numerical simulations and studies of the heat transfer and flow characteristics of microflows in fluidic MEMS. The present work demonstrates that the parallelized DSMC and Burnett equations are accurate methods for simulating the microflows in the continuum-transition regime. There are still some remaining technical issues that should be resolved to further advance the microflow simulation research. In the following, they are discussed briefly in the order of DSMC, Burnett equations, and a hybrid approach consisting of DSMC and Burnett equations.

DSMC

The current PDSMC code considers the molecules as polyatomic gas mixtures. Future DSMC improvements include the ability to handle more realistic flows with more complex geometries and plasma.

The MEMS geometries of practical interests often contain irregular shapes and
obstacles. The current PDSMC tool allows only structured uniform field-cells. The field-cells need to be replaced with unstructured cells. In MEMS applications, there may exist plasma and electric/magnetic fields. The electric force needs to be considered based on the plasma physics and electrodynamics.

**Burnett Equations**

Using the conventional Burnett equations, numerical instabilities can be encountered when simulating microchannel flows. The computational grid sizes cannot be much smaller than the mean-free-path of the gas being simulated. The Burnett solutions reported in this dissertation are for $Kn_c \leq 0.02$. Similar numerical instabilities were reported and analyzed in the simulation of hypersonic rarefied flows by Zhong (1991). The conventional Burnett equations are not stable for small wavelength perturbations; however, one can add the augmented Burnett terms, $\tau_y^{(a)}$ and $q_f^{(a)}$, to alleviate the numerical instabilities.

**A Hybrid of DSMC and Burnett Equations**

In many MEMS flows, strong rarefied gas effects usually exist in small regions near the surface. The flow in the remaining flow domain is either in the continuum or the slip-flow regimes. Due to this mixed flow regime character, a combined DSMC/Burnett modeling approach can be developed for MEMS flow calculations. In the small $Kn$ region, the Burnett equations solver is applied, and DSMC is used in the high $Kn$ region.
Appendix A

Acceptance-Rejection Method
Probability modeling of physical processes requires the generation of representative values of variables that are distributed in a prescribed manner. This is done through random numbers and is a key step in DSMC procedures.

*Acceptance-rejection* is one of the probabilistic algorithms usually used in DSMC simulations to generate representative values of variable $x$ that is distributed in a specific probability function $f_x$. The method assumes the existence of a set of successive random fractions, $R_t$, that are uniformly distributed between 0 and 1.

If the variable $x$ has a range from $a$ to $b$, the total probability is

$$
\int_a^b f_x \, dx = 1 \tag{A.1}
$$

The cumulative distribution function is defined as

$$
F_x = \int_a^x f_x \, dx \tag{A.2}
$$

If the distribution function $f_x$ is a constant of $1/(b-a)$, that is, $x$ is uniformly distributed between $a$ and $b$, a representative value of $x$ can be select by generating a random fraction $R_t$ and setting it equal to $F_x$ as

$$
F_x = R_t \tag{A.3}
$$

Equation (A.3) gives a representative value of $x$ by

$$
x = a + R_t(b-a) \tag{A.4}
$$

Unfortunately, it is impossible to invert equation (A.3) to obtain an explicit form of function like equation (A.4) for $x$ in a more realistic distribution of function $f_x$.

Alternatively, a representative value of $x$ can be generated by using the acceptance-
rejection algorithm through the following five steps:

Step 1: Normalize the distribution function $f_x$ by its maximum value $f_{\text{max}}$ to give

$$f'_x = f_x / f_{\text{max}}$$  \hspace{1cm} (A.5)

Step 2: Choose a value of $x$ at random on the basis of $x$ being uniformly distributed between its limits; i.e., from equation (A.4).

Step 3: Calculate the normalized distribution function $f'_x$ with the chosen $x$.

Step 4: Generate a second random fraction $R_r$.

Step 5: If $f'_x > R_r$, then accept the chosen $x$ and stop; otherwise, go back to step 2 and repeat the procedures until $x$ is accepted.

In a DSMC simulation, the velocity components and internal energy of a molecule are generated by the acceptance-rejection method from its specified velocity distribution function and internal energy distribution function, respectively, when initializing a molecule inside the computational domain or a molecule entering the computational domain, or taking account for a molecule reflected from a surface with the diffuse reflection model. The acceptance-rejection method is also used to determine collision pairs.
Appendix B

Coordinate Transformation
In the computation of Burnett equations, a finite difference method and a general body-fitted nonorthogonal grid are used. The governing equations (4.24-26) and the constitutive equation (4.53) written in Cartesian coordinate system \((x, y, z)\) are transformed into the general nonorthogonal computational coordinate system \((\xi, \eta, \zeta)\). The equations of the grid transformation are

\[
\begin{align*}
x &= x(\xi, \eta, \zeta) \\
y &= y(\xi, \eta, \zeta) \\
z &= z(\xi, \eta, \zeta)
\end{align*}
\]  

(B.1)

Applying the chain rule to equation (B.1) yields the first order transformation

\[
\begin{bmatrix}
\frac{\partial}{\partial x} \\
\frac{\partial}{\partial y} \\
\frac{\partial}{\partial z}
\end{bmatrix} =
\begin{bmatrix}
\xi_x & \eta_x & \zeta_x \\
\xi_y & \eta_y & \zeta_y \\
\xi_z & \eta_z & \zeta_z
\end{bmatrix}
\begin{bmatrix}
\frac{\partial}{\partial \xi} \\
\frac{\partial}{\partial \eta} \\
\frac{\partial}{\partial \zeta}
\end{bmatrix}
\]  

(B.2)

where \(\xi_x, \eta_x, \zeta_x, \xi_y, \eta_y, \zeta_y, \xi_z, \eta_z, \) and \(\zeta_z\) are the mesh metrics of first-order that will be derived in the following.

Taking the first order derivative of equation (B.1) with respect to \(x, y,\) and \(z,\) respectively, leads to

\[
\begin{bmatrix}
x_x & x_y & x_z \\
y_x & y_y & y_z \\
z_x & z_y & z_z
\end{bmatrix}
\begin{bmatrix}
\frac{\partial}{\partial \xi} \\
\frac{\partial}{\partial \eta} \\
\frac{\partial}{\partial \zeta}
\end{bmatrix} =
\begin{bmatrix}
1 \\
0 \\
0
\end{bmatrix}
\]  

(B.3a)

\[
\begin{bmatrix}
x_x & x_y & x_z \\
y_x & y_y & y_z \\
z_x & z_y & z_z
\end{bmatrix}
\begin{bmatrix}
\frac{\partial}{\partial \xi} \\
\frac{\partial}{\partial \eta} \\
\frac{\partial}{\partial \zeta}
\end{bmatrix} =
\begin{bmatrix}
0 \\
1 \\
0
\end{bmatrix}
\]  

(B.3b)
By solving the equations set of (B.3), the transformation Jacobian $J$ is,

$$J^{-1} = \frac{\partial (x, y, z)}{\partial (\xi, \eta, \zeta)} = x_{\xi} (y_{\zeta} z_{\zeta} - y_{\zeta} z_{\eta}) - x_{\eta} (y_{\zeta} z_{\zeta} - y_{\zeta} z_{\eta}) + x_{\zeta} (y_{\zeta} z_{\zeta} - y_{\zeta} z_{\eta})$$  \hspace{1cm} \text{(B.4)}$$

and the first order transformation metrics are given as

$$\xi_x = J(y_{\zeta} z_{\zeta} - y_{\zeta} z_{\eta})$$  \hspace{1cm} \text{(B.5a)}$$
$$\eta_x = J(y_{\zeta} z_{\zeta} - y_{\zeta} z_{\eta})$$  \hspace{1cm} \text{(B.5b)}$$
$$\zeta_x = J(y_{\zeta} z_{\zeta} - y_{\zeta} z_{\eta})$$  \hspace{1cm} \text{(B.5c)}$$
$$\xi_y = J(x_{\eta} z_{\eta} - x_{\eta} z_{\zeta})$$  \hspace{1cm} \text{(B.5d)}$$
$$\eta_y = J(x_{\eta} z_{\eta} - x_{\eta} z_{\zeta})$$  \hspace{1cm} \text{(B.5e)}$$
$$\zeta_y = J(x_{\eta} z_{\eta} - x_{\eta} z_{\zeta})$$  \hspace{1cm} \text{(B.5f)}$$
$$\xi_z = J(x_{\eta} y_{\eta} - x_{\eta} y_{\zeta})$$  \hspace{1cm} \text{(B.5g)}$$
$$\eta_z = J(x_{\eta} y_{\eta} - x_{\eta} y_{\zeta})$$  \hspace{1cm} \text{(B.5h)}$$
$$\zeta_z = J(x_{\eta} y_{\eta} - x_{\eta} y_{\zeta})$$  \hspace{1cm} \text{(B.5i)}$$

There are also second-order derivatives in the constitutive equation (4.53) for the viscous stress and heat flux terms. They can be obtained through the chain rule based on the first order transformations as,

$$\frac{\partial^2}{\partial x^2} = \xi_x^2 \frac{\partial^2}{\partial \xi^2} + \eta_x^2 \frac{\partial^2}{\partial \eta^2} + \zeta_x^2 \frac{\partial^2}{\partial \zeta^2} + 2\xi_x \eta_x \frac{\partial^2}{\partial \xi \partial \eta} + 2\xi_x \zeta_x \frac{\partial^2}{\partial \xi \partial \zeta} + 2\eta_x \zeta_x \frac{\partial^2}{\partial \eta \partial \zeta} + \xi_x \frac{\partial^2}{\partial \xi \partial \zeta} \frac{\partial}{\partial \zeta} + \eta_x \frac{\partial^2}{\partial \eta \partial \zeta} + \zeta_x \frac{\partial^2}{\partial \zeta \partial \zeta} \frac{\partial}{\partial \zeta}$$  \hspace{1cm} \text{(B.6)}$$
And the second-order mesh metrics can be obtained by taking further derivatives of equations (B.3a-3c) with respect to x, y, and z. For example, taking derivative of equation (B.3a) with respect to x yields,

\[
\frac{\partial^2}{\partial x^2} = \xi_x \frac{\partial^2}{\partial \xi^2} + \eta_x \frac{\partial^2}{\partial \eta^2} + \zeta_x \frac{\partial^2}{\partial \zeta^2} + 2 \xi_x \eta_x \frac{\partial^2}{\partial \xi \partial \eta} + 2 \xi_x \zeta_x \frac{\partial^2}{\partial \xi \partial \zeta} \\
+ 2 \eta_x \zeta_x \frac{\partial^2}{\partial \eta \partial \zeta} + \xi_x \frac{\partial}{\partial \xi} + \eta_x \frac{\partial}{\partial \eta} + \zeta_x \frac{\partial}{\partial \zeta}
\]  

(B.7)

\[
\frac{\partial^2}{\partial y^2} = \xi_y \frac{\partial^2}{\partial \xi^2} + \eta_y \frac{\partial^2}{\partial \eta^2} + \zeta_y \frac{\partial^2}{\partial \zeta^2} + 2 \xi_y \eta_y \frac{\partial^2}{\partial \xi \partial \eta} + 2 \xi_y \zeta_y \frac{\partial^2}{\partial \xi \partial \zeta} \\
+ 2 \eta_y \zeta_y \frac{\partial^2}{\partial \eta \partial \zeta} + \xi_y \frac{\partial}{\partial \xi} + \eta_y \frac{\partial}{\partial \eta} + \zeta_y \frac{\partial}{\partial \zeta}
\]  

(B.8)

\[
\frac{\partial^2}{\partial z^2} = \xi_z \frac{\partial^2}{\partial \xi^2} + \eta_z \frac{\partial^2}{\partial \eta^2} + \zeta_z \frac{\partial^2}{\partial \zeta^2} + 2 \xi_z \eta_z \frac{\partial^2}{\partial \xi \partial \eta} + 2 \xi_z \zeta_z \frac{\partial^2}{\partial \xi \partial \zeta} \\
+ 2 \eta_z \zeta_z \frac{\partial^2}{\partial \eta \partial \zeta} + \xi_z \frac{\partial}{\partial \xi} + \eta_z \frac{\partial}{\partial \eta} + \zeta_z \frac{\partial}{\partial \zeta}
\]  

(B.9)

\[
\frac{\partial^2}{\partial x \partial y} = \xi_x \xi_y \frac{\partial^2}{\partial \xi \partial \eta} + (\xi_x \eta_y + \eta_x \xi_y) \frac{\partial^2}{\partial \xi \partial \eta} + \xi_y \zeta_x \frac{\partial}{\partial \xi} + \eta_y \zeta_x \frac{\partial}{\partial \eta} + \zeta_y \zeta_x \frac{\partial}{\partial \zeta}
\]  

(B.10)

\[
\frac{\partial^2}{\partial x \partial z} = \xi_x \xi_z \frac{\partial^2}{\partial \xi \partial \zeta} + (\xi_x \eta_z + \eta_x \xi_z) \frac{\partial^2}{\partial \eta \partial \zeta} + \xi_z \zeta_x \frac{\partial}{\partial \xi} + \eta_z \zeta_x \frac{\partial}{\partial \eta} + \zeta_z \zeta_x \frac{\partial}{\partial \zeta}
\]  

(B.11)

\[
\frac{\partial^2}{\partial y \partial z} = \xi_y \xi_z \frac{\partial^2}{\partial \eta \partial \zeta} + (\xi_y \eta_z + \eta_y \xi_z) \frac{\partial^2}{\partial \eta \partial \zeta} + \xi_z \zeta_y \frac{\partial}{\partial \xi} + \eta_z \zeta_y \frac{\partial}{\partial \eta} + \zeta_z \zeta_y \frac{\partial}{\partial \zeta}
\]  

(B.12)

with

\[
(\xi_x \eta_y + \eta_x \xi_y) \frac{\partial^2}{\partial \xi \partial \eta} + \xi_y \zeta_x \frac{\partial}{\partial \xi} + \eta_y \zeta_x \frac{\partial}{\partial \eta} + \zeta_y \zeta_x \frac{\partial}{\partial \zeta}
\]  

(B.13a)

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and the final results for the second-order mesh metric with respect to $x$ are,

\[ \xi_{xx} = -(a_1 \xi_x + b_1 \xi_y + c_1 \xi_z) \]  
(B.14)

\[ \eta_{xx} = -(a_2 \eta_x + b_2 \eta_y + c_2 \eta_z) \]  
(B.15)

\[ \zeta_{xx} = -(a_3 \zeta_x + b_3 \zeta_y + c_3 \zeta_z) \]  
(B.16)

where

\[ a_1 = x_{\xi\xi} \xi_x^2 + x_{\eta\eta} \eta_x^2 + x_{\zeta\zeta} \zeta_x^2 + 2 x_{\xi\eta} \xi_x \eta_x + 2 x_{\xi\zeta} \xi_x \zeta_x + 2 x_{\eta\zeta} \eta_x \zeta_x \]  

\[ b_1 = y_{\xi\xi} \xi_x^2 + y_{\eta\eta} \eta_x^2 + y_{\zeta\zeta} \zeta_x^2 + 2 y_{\xi\eta} \xi_x \eta_x + 2 y_{\xi\zeta} \xi_x \zeta_x + 2 y_{\eta\zeta} \eta_x \zeta_x \]  

\[ c_1 = z_{\xi\xi} \xi_x^2 + z_{\eta\eta} \eta_x^2 + z_{\zeta\zeta} \zeta_x^2 + 2 z_{\xi\eta} \xi_x \eta_x + 2 z_{\xi\zeta} \xi_x \zeta_x + 2 z_{\eta\zeta} \eta_x \zeta_x \]  

Similarly, the other mesh metrics of second-order are,

\[ \xi_{yy} = -(a_2 \xi_x + b_2 \xi_y + c_2 \xi_z) \]  
(B.17)

\[ \eta_{yy} = -(a_2 \eta_x + b_2 \eta_y + c_2 \eta_z) \]  
(B.18)

\[ \zeta_{yy} = -(a_2 \zeta_x + b_2 \zeta_y + c_2 \zeta_z) \]  
(B.19)

where

\[ a_2 = x_{\xi\xi} \xi_y^2 + x_{\eta\eta} \eta_y^2 + x_{\zeta\zeta} \zeta_y^2 + 2 x_{\xi\eta} \xi_y \eta_y + 2 x_{\xi\zeta} \xi_y \zeta_y + 2 x_{\eta\zeta} \eta_y \zeta_y \]  

\[ b_2 = y_{\xi\xi} \xi_y^2 + y_{\eta\eta} \eta_y^2 + y_{\zeta\zeta} \zeta_y^2 + 2 y_{\xi\eta} \xi_y \eta_y + 2 y_{\xi\zeta} \xi_y \zeta_y + 2 y_{\eta\zeta} \eta_y \zeta_y \]  

\[ c_2 = z_{\xi\xi} \xi_y^2 + z_{\eta\eta} \eta_y^2 + z_{\zeta\zeta} \zeta_y^2 + 2 z_{\xi\eta} \xi_y \eta_y + 2 z_{\xi\zeta} \xi_y \zeta_y + 2 z_{\eta\zeta} \eta_y \zeta_y \]  

\[ \xi_{zz} = -(a_3 \xi_x + b_3 \xi_y + c_3 \xi_z) \]  
(B.20)
\[
\eta_a = -(a_a \eta_x + b_a \eta_y + c_a \eta_z) \tag{B.22}
\]
\[
\zeta_a = -(a_a \zeta_x + b_a \zeta_y + c_a \zeta_z) \tag{B.23}
\]

where

\[
a_3 = x_{33} \xi_z^2 + x_{33} \eta_z + x_{33} \zeta_z \xi_z + x_{33} (\xi_z \eta_z + \xi_z \eta_z) + x_{33} (\xi_z \zeta_z + \xi_z \zeta_z) + x_{33} (\eta_z \zeta_z + \eta_z \zeta_z)
\]
\[
b_3 = y_{33} \xi_z^2 + y_{33} \eta_z + y_{33} \zeta_z \xi_z + y_{33} (\xi_z \eta_z + \xi_z \eta_z) + y_{33} (\xi_z \zeta_z + \xi_z \zeta_z) + y_{33} (\eta_z \zeta_z + \eta_z \zeta_z)
\]
\[
c_3 = z_{33} \xi_z^2 + z_{33} \eta_z + z_{33} \zeta_z \xi_z + z_{33} (\xi_z \eta_z + \xi_z \eta_z) + z_{33} (\xi_z \zeta_z + \xi_z \zeta_z) + z_{33} (\eta_z \zeta_z + \eta_z \zeta_z)
\]
\[
\xi \zeta = -(a_s \xi_x + b_s \xi_y + c_s \xi_z) \tag{B.24}
\]
\[
\eta \zeta = -(a_s \eta_x + b_s \eta_y + c_s \eta_z) \tag{B.25}
\]
\[
\zeta \zeta = -(a_s \zeta_x + b_s \zeta_y + c_s \zeta_z) \tag{B.26}
\]

where

\[
a_4 = x_{44} \xi_x^2 + x_{44} \eta_x + x_{44} \zeta_x \xi_x + x_{44} (\xi_x \eta_x + \xi_x \eta_x) + x_{44} (\xi_x \zeta_x + \xi_x \zeta_x) + x_{44} (\eta_x \zeta_x + \eta_x \zeta_x)
\]
\[
b_4 = y_{44} \xi_x^2 + y_{44} \eta_x + y_{44} \zeta_x \xi_x + y_{44} (\xi_x \eta_x + \xi_x \eta_x) + y_{44} (\xi_x \zeta_x + \xi_x \zeta_x) + y_{44} (\eta_x \zeta_x + \eta_x \zeta_x)
\]
\[
c_4 = z_{44} \xi_x^2 + z_{44} \eta_x + z_{44} \zeta_x \xi_x + z_{44} (\xi_x \eta_x + \xi_x \eta_x) + z_{44} (\xi_x \zeta_x + \xi_x \zeta_x) + z_{44} (\eta_x \zeta_x + \eta_x \zeta_x)
\]
\[
\xi \zeta = -(a_s \xi_x + b_s \xi_y + c_s \xi_z) \tag{B.27}
\]
\[
\eta \zeta = -(a_s \eta_x + b_s \eta_y + c_s \eta_z) \tag{B.28}
\]
\[
\zeta \zeta = -(a_s \zeta_x + b_s \zeta_y + c_s \zeta_z) \tag{B.29}
\]

where

\[
a_5 = x_{55} \xi_z^2 + x_{55} \eta_z + x_{55} \zeta_z \xi_z + x_{55} (\xi_z \eta_z + \xi_z \eta_z) + x_{55} (\xi_z \zeta_z + \xi_z \zeta_z) + x_{55} (\eta_z \zeta_z + \eta_z \zeta_z)
\]
\[
b_5 = y_{55} \xi_z^2 + y_{55} \eta_z + y_{55} \zeta_z \xi_z + y_{55} (\xi_z \eta_z + \xi_z \eta_z) + y_{55} (\xi_z \zeta_z + \xi_z \zeta_z) + y_{55} (\eta_z \zeta_z + \eta_z \zeta_z)
\]
\[ c = z_{\xi} \xi + z_{\eta} \eta + z_{\zeta} \zeta + x_{\xi} (\xi, \eta_{1} + \xi, \eta_{2}) + x_{\eta} (\eta_{1} + \xi, \eta_{2}) + x_{\zeta} (\xi, \eta_{1} + \xi, \eta_{2}) \]

\[ \xi_{y} = -(a_{0} \xi_{x} + b_{0} \xi_{y} + c_{0} \xi_{z}) \quad (B.30) \]

\[ \eta_{y} = -(a_{0} \eta_{x} + b_{0} \eta_{y} + c_{0} \eta_{z}) \quad (B.31) \]

\[ \zeta_{y} = -(a_{0} \zeta_{x} + b_{0} \zeta_{y} + c_{0} \zeta_{z}) \quad (B.32) \]

where

\[ a_{0} = x_{\xi} \xi_{x} + x_{\eta} \eta_{x} + x_{\zeta} \zeta_{x} + x_{\xi} (\xi, \eta_{1} + \xi, \eta_{2}) + x_{\eta} (\eta_{1} + \xi, \eta_{2}) + x_{\zeta} (\xi, \eta_{1} + \xi, \eta_{2}) \]

\[ b_{0} = y_{\xi} \xi_{y} + y_{\eta} \eta_{y} + y_{\zeta} \zeta_{y} + y_{\xi} (\xi, \eta_{1} + \xi, \eta_{2}) + y_{\eta} (\eta_{1} + \xi, \eta_{2}) + y_{\zeta} (\xi, \eta_{1} + \xi, \eta_{2}) \]

\[ c_{0} = z_{\xi} \xi_{z} + z_{\eta} \eta_{z} + z_{\zeta} \zeta_{z} + z_{\xi} (\xi, \eta_{1} + \xi, \eta_{2}) + z_{\eta} (\eta_{1} + \xi, \eta_{2}) + z_{\zeta} (\xi, \eta_{1} + \xi, \eta_{2}) \]
Appendix C

Jacobian Matrices
The inviscid Jacobian matrices are given by

\[
A = \begin{bmatrix}
\frac{\partial C}{\partial Q} & \rho \alpha_1 & \rho \alpha_2 & \rho \alpha_3 & \frac{\rho U}{h} \\
\frac{\partial C}{\partial Q} & \rho (U + \alpha_1 u) & \rho u \alpha_1 & \rho u \alpha_2 & \rho u \alpha_3 & \frac{\rho u U}{h} \\
\frac{\partial C}{\partial Q} & \rho (U + \alpha_2 v) & \rho v \alpha_1 & \rho v \alpha_2 & \rho v \alpha_3 & \frac{\rho v U}{h} \\
\frac{\partial C}{\partial Q} & \rho (U + \alpha_3 w) & \rho w \alpha_1 & \rho w \alpha_2 & \rho w \alpha_3 & \frac{\rho w U}{h} \\
\frac{\partial C}{\partial Q} & \rho (u + \alpha_1 H) & \rho (vU + \alpha_2 H) & \rho (wU + \alpha_3 H) & \rho U (1 - H) \\
\frac{\partial C}{\partial Q} & \rho (u + \alpha_2 H) & \rho (vU + \alpha_3 H) & \rho (wU + \alpha_1 H) & \rho U (1 - H) \\
\end{bmatrix}
\]

\[
B = \begin{bmatrix}
\frac{\partial C}{\partial Q} & \rho \alpha_1 & \rho \alpha_2 & \rho \alpha_3 & \frac{\rho U}{h} \\
\frac{\partial C}{\partial Q} & \rho (U + \alpha_1 u) & \rho u \alpha_1 & \rho u \alpha_2 & \rho u \alpha_3 & \frac{\rho u U}{h} \\
\frac{\partial C}{\partial Q} & \rho (U + \alpha_2 v) & \rho v \alpha_1 & \rho v \alpha_2 & \rho v \alpha_3 & \frac{\rho v U}{h} \\
\frac{\partial C}{\partial Q} & \rho (U + \alpha_3 w) & \rho w \alpha_1 & \rho w \alpha_2 & \rho w \alpha_3 & \frac{\rho w U}{h} \\
\frac{\partial C}{\partial Q} & \rho (u + \alpha_2 H) & \rho (vU + \alpha_3 H) & \rho (wU + \alpha_1 H) & \rho U (1 - H) \\
\frac{\partial C}{\partial Q} & \rho (u + \alpha_3 H) & \rho (vU + \alpha_1 H) & \rho (wU + \alpha_2 H) & \rho U (1 - H) \\
\end{bmatrix}
\]

\[
C = \begin{bmatrix}
\frac{\partial C}{\partial Q} & \rho \alpha_1 & \rho \alpha_2 & \rho \alpha_3 & \frac{\rho U}{h} \\
\frac{\partial C}{\partial Q} & \rho (U + \alpha_1 u) & \rho u \alpha_1 & \rho u \alpha_2 & \rho u \alpha_3 & \frac{\rho u U}{h} \\
\frac{\partial C}{\partial Q} & \rho (U + \alpha_2 v) & \rho v \alpha_1 & \rho v \alpha_2 & \rho v \alpha_3 & \frac{\rho v U}{h} \\
\frac{\partial C}{\partial Q} & \rho (U + \alpha_3 w) & \rho w \alpha_1 & \rho w \alpha_2 & \rho w \alpha_3 & \frac{\rho w U}{h} \\
\frac{\partial C}{\partial Q} & \rho (u + \alpha_1 H) & \rho (vU + \alpha_2 H) & \rho (wU + \alpha_3 H) & \rho U (1 - H) \\
\frac{\partial C}{\partial Q} & \rho (u + \alpha_2 H) & \rho (vU + \alpha_3 H) & \rho (wU + \alpha_1 H) & \rho U (1 - H) \\
\end{bmatrix}
\]

where

\[
U = \alpha_1 u + \alpha_2 v + \alpha_3 w
\]

\[
\alpha_1 = \xi_s, \quad \alpha_2 = \xi_y, \quad \alpha_3 = \xi_z
\]

here $C_p$ is the specific heat. The Jacobian $B$ is obtained by setting $\alpha_1 = \eta_s, \alpha_2 = \eta_y,$ and $\alpha_3 = \eta_z$; and the Jacobian $C$ is obtained by setting $\alpha_1 = \xi_s, \alpha_2 = \xi_y$, and $\alpha_3 = \xi_z$. 

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The viscous Jacobians, $R_{zz} = \frac{\partial \tilde{F}_z}{\partial \tilde{Q}}$, $R_{\eta\eta} = \frac{\partial \tilde{F}_\eta}{\partial \tilde{Q}}$ and $R_{\zeta\zeta} = \frac{\partial \tilde{G}_\zeta}{\partial \tilde{Q}}$ has the following form

$$
R_{zz} = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & \mu \left( \frac{1}{3} \alpha_1^2 + \Lambda \right) & \mu \alpha_{12} & \mu \alpha_{13} & 0 \\
0 & \rho \nu \alpha_{1} & \mu \left( \frac{1}{3} \alpha_2^2 + \Lambda \right) & \mu \alpha_{23} & 0 \\
0 & \mu \alpha_{13} & \mu \alpha_{23} & \mu \left( \frac{1}{3} \alpha_3^2 + \Lambda \right) & 0 \\
0 & \pi_u & \pi_v & \pi_w & \frac{\mu \Lambda}{Pr}
\end{bmatrix} \tag{C.8}
$$

where

$$
\alpha_1 = \xi_1, \quad \alpha_2 = \xi_2, \quad \alpha_3 = \xi_3, \\
\alpha_{12} = \frac{1}{3} \alpha_1 \alpha_2, \quad \alpha_{13} = \frac{1}{3} \alpha_1 \alpha_3, \\
\alpha_{23} = \frac{1}{3} \alpha_2 \alpha_3, \quad \Lambda = \alpha_1^2 + \alpha_2^2 + \alpha_3^2, \\
\pi_u = \mu \left[ u \left( \frac{1}{3} \alpha_1^2 + \Lambda \right) + \nu \alpha_{12} + w \alpha_{13} \right], \\
\pi_v = \mu \left[ v \left( \frac{1}{3} \alpha_2^2 + \Lambda \right) + u \alpha_{12} + w \alpha_{23} \right], \tag{C.9}
$$

$$
\pi_w = \mu \left[ w \left( \frac{1}{3} \alpha_3^2 + \Lambda \right) + u \alpha_{13} + v \alpha_{23} \right]
$$

$R_{\eta\eta}$ is also obtained by set $\alpha_1 = \eta_1$, $\alpha_2 = \eta_2$ and $\alpha_3 = \eta_3$ and $R_{\zeta\zeta}$ is obtained by setting $\alpha_1 = \zeta_1$, $\alpha_2 = \zeta_2$ and $\alpha_3 = \zeta_3$. 

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