MODELING OF MICROSCALE GAS FLOWS USING THE DIRECT SIMULATION MONTE CARLO METHOD

A Thesis in
Aerospace Engineering

by
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Abstract

Microflows are defined as fluid flow phenomena associated with microscale mechanical devices. A great number of such devices have been manufactured over the last few decades using surface and bulk silicon micro-machining. Many of micro-electromechanical systems (MEMS) involve gaseous flows. Gas flows in MEMS with characteristic size on the order of microns differ from their larger counterparts. Three important flow parameters: Knudsen and Reynolds numbers and surface-to-volume ratio, are drastically different from those encountered in large scale flows. Accurate numerical modeling of microflows is indispensable for providing design capability for MEMS by predicting the flow field and performance characteristics. The main goal of the thesis research is the development, implementation and application of comprehensive direct simulation Monte Carlo approach to microscale gas flows.

Flows in microthrusters and microchannels are commonly encountered in MEMS and are the focus of the study. The investigation of physical processes in three-dimensional micronozzles and the influence of Reynolds number, geometrical configuration and temperature regime have been carried out in the thesis. The impact of wall effects on thrust is examined for axisymmetric and two- and three-dimensional cold gas micronozzles. The flow in a flat micronozzle has a 3D structure and is strongly influenced by the end walls. The additional friction losses on the side walls cause a reduction in thrust of about 20% compared to the two-dimensional and axisymmetric nozzles.
The work on coupled analysis of a microthruster is aimed at developing a numerical simulation code capable of modeling the temporal variation of microthruster material temperature and performance characteristics. The application of the developed approach to two-dimensional and three-dimensional microthrusters gives several important insights into the dependence of performance characteristics on Reynolds number, thermal conditions and thruster geometry. The mass discharge of the microthruster have been found to decrease significantly in time due to increasing wall temperature. Such behavior of the mass discharge coefficient is obtained for both 2D and 3D models as well as for different stagnation pressures and geometrical shapes.

Investigation of gas flows in microchannels with constriction have been carried out both analytically and numerically in order to understand the flow phenomena observed in experiments. An analytical model is developed to predict pressure drop and mass flow rate. The validation of the model is conducted by comparison with 2D DSMC calculations. The model accurately predicts the mass flow rate and pressure drop at the constriction section and compares well with the DSMC results. The DSMC simulations have shown that the flow separation may occur at the constriction. The presence of the separation zone does not influence the pressure distribution and the mass flow rate.

The DSMC method have been applied for calibration of micro-Newton thrust stand and investigation of effects of the facility background. The DSMC calculations have been conducted for orifice flow for $Kn = 0.01$ to 40. It is found that for low Knudsen numbers the background gas contribution to the total force becomes significant. This is attributed to the jet shadowing effect, and, therefore, it must be included in modeling to permit a comparison with experiment.
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Nomenclature

\( A \) - area

\( a \) - speed of sound

\( \bar{c} \) - mean thermal speed

\( c_d \) - mass discharge coefficient

\( c_p \) - specific heat at constant pressure

\( d \) - diameter, depth

\( F \) - force

\( g \) - magnitude of relative velocity of colliding particles

\( h \) - height

\( I_{sp} \) - specific impulse

\( Kn \) - Knudsen number

\( k \) - thermal conductivity

\( L \) - characteristic length

\( M \) - Mach number

\( N_\lambda \) - number of particles in a volume with linear size equal to the local mean free path

\( \dot{m} \) - mass flux

\( p \) - pressure

\( R \) - gas constant

\( Re \) - Reynolds number

\( s \) - speed ratio
$T$ - temperature

$u$ - X-component of velocity

$\Delta t$ - time step

**Greek:**

$\alpha_t$ - tangential momentum accommodation coefficient

$\alpha_E$ - energy accommodation coefficient

$\gamma$ - specific heat ratio

$\lambda$ - molecular mean free path

$\mu$ - dynamic viscosity

$\nu$ - kinematic viscosity

$\Omega$ - domain

$\rho$ - density

$\sigma$ - differential collision cross-section

$\tau$ - characteristic time

$\chi$ - scattering angle

**Subscripts:**

$0$ - stagnation chamber

$b$ - background gas

$e$ - domain boundary, exit

$g$ - gas

$in$ - inlet
int - interior

j - jet

out - outlet

s - solid

t - throat

un - uniform channel

w - wall

Superscripts:

* - ideal vacuum conditions

+, - - opposite plenum surfaces

t - transposed
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Chapter 1

Introduction

1.1 Microflows

Microflows are defined as fluid flow phenomena associated with micro-scale devices. A great number of such mechanical devices have been manufactured over the last few decades when such micro-manufacturing techniques as surface and bulk silicon micro-machining have been developed. Micro-electro-mechanical systems (MEMS) is the integration of mechanical elements, sensors, actuators, and electronics on a common silicon substrate through micro-fabrication technology. Not all MEMS devices involve gaseous flows but a multitude of them do, for example, microducts, micropumps, microturbines and microvalves.

The fluid mechanics of microdevices has become an area of active research in the last decade and recently a first monograph [48] in the field have been published. Fluid flows in small devices with characteristic size on the order of microns differ from those in their large scale counterparts. Three important flow parameters: Knudsen and Reynolds numbers and the surface-to-volume ratio that define flow regime, are drastically different from what is commonly encountered in macroscale flows. Many of the MEMS devices use gases at standard atmospheric conditions as the working fluids and, since the characteristic length scale is in the sub-micron range, the molecular effects become important.
Knudsen number defined as the ratio of the molecular mean free path to the characteristic length scale characterizes the influence of molecular effects. The classification of flow rarefaction regimes based on the Knudsen number was first proposed in Ref. [83] and is given in Fig. 1.1 where also the applicable governing equations for each flow regime are indicated.

Fig. 1.1. Flow rarefaction regimes based on Knudsen number and governing equations.

For air at standard room temperature of 287 K and pressure of 101.3 kPa, the mean free path is approximately 52 nanometers. Thus, a device which involves a flow section with characteristic length of 1 micron, and air at standard conditions, would have a Knudsen number of $5.2 \times 10^{-2}$. That means that the flow is in the slip regime, a regime of slight rarefaction where the gas might exhibit some characteristics of its coarse molecular structure near solid wall boundaries. If the characteristic size is a tenth of a micron or the characteristic pressure is a tenth of atmosphere, then the Knudsen number
is 0.5 and the flow is in the transitional regime between slip and free molecular flow. In the transitional regime intermolecular and surface collisions are of equal importance. At a nanometer scale device the flow may become free molecular and here the flow phenomena are governed by molecule-surface collisions. Due to large pressure gradients in MEMS devices, several regimes of rarefaction may be encountered simultaneously in different parts of the flow domain.

Another important non-dimensional parameter for microflows is the Reynolds number that characterizes the ratio of inertial to viscous forces:

$$Re = \frac{LU}{\nu}$$

The Reynolds number in micro devices is also affected by the extremely small length scale. From the kinetic theory, the kinematic viscosity coefficient $\nu$ can be expressed as \[77\]:

$$\nu = \frac{\lambda \bar{c}}{2}$$

where $\bar{c}$ is the mean thermal speed, $\bar{c} = \sqrt{\frac{8}{\pi}RT}$. Hence, one can relate the Reynolds number to the Mach and Knudsen numbers:

$$Re = \frac{M}{Kn} \sqrt{\frac{\pi \gamma}{2}}.$$

The flows in MEMS devices are usually in subsonic to transonic regime. Thus, the characteristic velocity scale is usually a fraction of the speed of sound $a = \sqrt{\gamma RT}$. For air at standard conditions in a 1 micron length scale device and a Mach number
of 1, the Reynolds number is approximately 23. Therefore, microflows are typically in the regime when viscous effects play a very significant role. If the length scale is further diminished to nanometers, the flow will be in “creeping” regime with $Re << 1$.

The third parameter that characterizes microscale flows and distinguishes them from their macroscopic analogues is the increased surface-to-volume ratio. Clearly, the ratio varies inversely proportional to the linear size. For example, in a micron sized device there is a million-fold increase in the surface-to-volume ratio compared to a device of 1 meter characteristic length. Therefore, in microscale devices fluid flows are dominated by surface effects. Surface friction and heat transfer are the two main loss factors in microscale devices [28]. The increase in the surface-to-volume ratio implies a proportional increase in the rate at which heat is transferred to a microscale device. Hence, the time to cool down or heat up a microscale device can be very small.

The rapid progress in developing of manufacturing techniques for microdevices has not been accompanied yet with the same level of understanding of the fluid mechanics of microflows. The experimental measurements are very difficult to make at such small scale. When using conventional techniques for conducting measurements on MEMS components, usually, errors become very large. One soon realizes that the measuring tools have to be even smaller in size than the object on which such measurements are made. The ability to model microflows numerically with high accuracy is indispensable. Numerical modeling of microflows can provide design capability for MEMS devices by predicting definitely the flow field and performance characteristics.
1.2 Modeling approach: DSMC

The three main factors: rarefaction (high Knudsen number), viscosity (low Reynolds number), and the dominance of the surface effects (large surface-to-volume ratio) are needed to be taken into account in numerical modeling of microflows.

For small Knudsen numbers the continuum hypothesis is: flow parameters such as density and velocity can be defined as averages over elements large enough in comparison to the microscopic structure of the gas, but small enough in comparison to the scale of macroscopic flow phenomena. In this case and when the flow is not far from thermodynamic equilibrium, the numerical modeling is based on the numerical solution of Euler equations for inviscid or Navier-Stokes equations for viscous flows.

For Knudsen numbers larger than 0.01, the non-equilibrium rarefaction influences the flow near gas-solid interfaces. These effects can be accounted for in the boundary conditions for Navier-Stokes equations as first-order approximations in Knudsen number velocity slip and temperature jump conditions. The former boundary condition was first obtained by Maxwell [63]. For the flows with Knudsen number larger than 0.1, the higher-order kinetic effects become important and the linear stress-strain relationships in Navier-Stokes equations become invalid. Burnett equations [22] which can be obtained from the Chapman-Enskog expansion of the Boltzmann equation to the second-order in Knudsen number can be used as governing equations in transitional regime. However, instability problems inherent in Burnett equations [17] lead to many numerical difficulties and require additional reformulation [1]. Eventually, when the Knudsen number is further
increased and the flow deviates significantly from equilibrium, the modeling has to be based on the Boltzmann equation, the principal equation of the kinetic theory.

The exact solution of the Boltzmann equation is available only for a limited number of special cases of collisionless flows or simple geometries [18, 23, 52]. For the problems of non-equilibrium gas flows involving complex geometries the main line of attack is to obtain numerical solutions of the Boltzmann equation. A survey of numerical methods for Boltzmann equation can be found in Ref. [7]. Generally, numerical solutions for the Boltzmann equation fall into one of the two categories: direct numerical integration of the Boltzmann equation or particle simulation. The direct numerical integration of the Boltzmann equation, which is sometimes referred as direct Boltzmann CFD, employs finite difference or finite element discretization of the velocity distribution function. The direct integration methods use either deterministic or Monte Carlo techniques for evaluation of the collision integral in the right-hand side of the Boltzmann equation. The large number of independent variables (four variables are required for a steady one-dimensional flow) and high computational cost of calculation of the collision integral impedes the practical application of the direct Boltzmann CFD methods.

The alternative group of numerical methods for solution of the Boltzmann equation is based on the direct statistical simulation of the molecular processes described by the kinetic theory. These methods most often attempt to treat a gas flow in physical terms as a collection of particles. This approach is used in the formulation of the direct simulation Monte Carlo (DSMC) method. The fundamental principle of the DSMC method is the splitting of the continuous motion of gas molecules during a time interval $\Delta t$ into two sequential stages: free-molecule flight and collisions. The DSMC method is
non-stationary in nature, but can be used to solve stationary problems with the following procedure. In the entire computational domain an arbitrary initial state of the gas is specified and given boundary conditions are imposed. A steady flow is obtained as the large time state of the unsteady flow.

In the DSMC method the physical flow domain is discretized into a grid of cells. Structured and unstructured grids can be used in DSMC calculations. In both cases, the size of grid cells should be sufficiently small so that the change in gas dynamic properties across each cell is small. In other words, the Knudsen number based on the cell size should be larger than one to allow accurate calculation of particle collisions. When the cell size in a simulation is too big, macroscopic gradients are typically under-predicted and the solution corresponds to an artificially larger Knudsen number. The time step in the simulation is usually selected as $\Delta t = \min(\tau_\lambda, \tau_{res})$, where $\tau_\lambda$ is the mean time between collisions, $\tau_{res}$ is the mean residence time in a cell, so that the molecules do not cross more than one cell during a time step. After steady flow is reached, sampling of macroparameters within each cell is performed for a large number of time steps to minimize the statistical scatter.

The advantages of using the DSMC method to study multi-dimensional microscale gas flows involving multi-component mixtures of non-perfect gases are: comparative simplicity of implementation even in three-dimensional form; the possibility of using various physical models for particle interactions, internal energy transfer and chemical reactions, and the ability to apply the method on modern parallel computers.
1.3 Challenges of DSMC modeling of microflows

Application of the DSMC method for modeling of microflows is complicated by a number of numerical and physical factors. First, the gas flows in micro-electromechanical systems are inherently three-dimensional. This is because the geometric shape of a mechanical device is chosen to maximize the performance while minimizing the cost of manufacture. For the fabrication of MEMS devices the technique is well developed for etching a simple-shaped device from a plane silicon wafer. As a result, the gas flow in such devices are three-dimensional and the performance prediction based on two-dimensional modeling can lead to significant design errors. Three-dimensional modeling and effective implementation of the DSMC method to handle complex geometries is therefore needed.

Second, in microscale devices the flow parameters are often known at the domain inlet and outlet boundaries in the form of stagnation pressure and temperature for microthrusters, or inlet and outlet pressure and temperature for microchannels. The boundary conditions in the DSMC method need to be specified in terms of number flux, temperature and mean flow velocity. In a supersonic inflow/outflow boundary these three flow quantities can be imposed freely. In micronozzle and microchannel flows the inlet and often outlet flow boundaries have to be in a subsonic region. Therefore, modeling of such flows will require the application of implicit boundary conditions.

Third, in many microflow applications the wall temperature is a major control factor affecting the gas flowfield and the overall device performance. The temporal and spatial distribution of the surface temperature is determined by the heat transfer between
the gas and the solid surface. In microdevices, the coupling between the heat transfer in
the solid and the gas flow exists and has to be properly modeled.

Fourth, since the flows in microdevices are often both in the near-continuum and
transitional regimes, the application of the DSMC method requires substantial computa-
tional resources. For this reason, statistical dependence indicators have to be applied
during the DSMC calculation in order to estimate and avoid significant numerical errors.

1.4 Objectives of the work

The main goal of the proposed thesis research is the development, implementation
and application of a comprehensive DSMC modeling approach to microscale gas flows.
The flows in microthrusters and microchannels are frequently encountered in MEMS
devices and are, therefore, the focus of the study.

In order to obtain reliable results for the flow structure and performance character-
istics in MEMS applications using the DSMC method, several additions to the standard
technique are required. In particular, it is necessary to apply an implicit subsonic inlet
boundary conditions in the DSMC method to accurately predict microchannel flows. In
the near continuum flow regime, DSMC calculations require very large computational
resources and parallel implementation of the DSMC algorithm becomes indispensable.
Finally, when the flow conditions are not adiabatic and the wall temperature is unknown,
the DSMC simulation has to be coupled with a transient conduction heat transfer anal-
ysis.
1.5 Thesis structure

The structure of the thesis is as follows. Chapter 2 focuses on the important issues related to the direct statistical simulation such as underlying assumptions, applicability, accuracy, and the speed of convergence. The connection between the master kinetic equation and the Boltzmann equation is discussed for a spatially uniform case. Next, we follow the construction of the exact statistical simulation algorithm for the solution of the N-particle equation. The two approximate numerical schemes for collisional relaxation most commonly used in the direct simulation Monte Carlo method are described.

Chapter 3 focuses on the numerical study of viscous effects in cold and high-temperature gas micronozzle flows and comparison of different geometric configurations, axisymmetric conical and flat three-dimensional, in terms of thrust performance and flow fields. A two-dimensional model of a micronozzle is also examined and compared with the full three-dimensional simulation in this chapter. The effects of the temperature regime on micronozzle performance are analyzed and the results of DSMC simulations are validated by comparison with experimental data.

The thermal coupling between solid walls and high-temperature gas in a three-dimensional microthruster is studied in Chapter 4. First, the proposed approach to coupled thermal and fluid analysis of high-temperature gas microthruster is described. Then the results of the numerical study of the effects of flow three-dimensionality, Reynolds number, and wall cooling conditions on the performance of a prototype thruster are presented and discussed.
Chapter 5 is devoted to the study of gas flows in microchannels with constrictions. Analytical model for prediction of mass flow rate and pressure distribution is presented and compared with numerical simulations using the DSMC method. The DSMC simulations are also used to investigate the possibility of flow separation in the constriction section.

An application of DSMC technique for micropropulsion testing is presented in Chapter 6. The DSMC method is applied to model a rarefied gas expansion through a thin circular orifice. The numerical and experimental results obtained outside of the thesis are used to calibrate a torsional thrust stand designed to measure force levels of micro- and milli-Newton.

Chapter 7 outlines the conclusions drawn from the thesis research.
Chapter 2

Direct Simulation Monte Carlo method

2.1 Mathematical foundations of DSMC method

The direct simulation Monte Carlo method is frequently described as a phenomenological approach for simulation of rarefied gas flows by modeling the motion of fictitious particles. The phenomenological description of the method is not necessary and can obscure the important issues related to the direct statistical simulation such as the underlying assumptions, applicability, accuracy and the speed of convergence.

The construction of the direct statistical simulation algorithm which lies in the basis of DSMC method is derived from several results of the kinetic theory. In this chapter, first, the derivation of the N-particle master kinetic equation is given following Ref. [75]. Then the connection between the master kinetic equation and the Boltzmann equation is discussed for spatially uniform case. Next, we follow the construction of the exact statistical simulation algorithm in section 2.2 for the solution of the N-particle equation. Finally, we compare the two widely used approximate numerical schemes for the collisional relaxation used in the direct simulation Monte Carlo method.

2.1.1 The master kinetic equation

The derivation of the N-particle master kinetic equation follows the derivation of master equation for one stochastic variable in Ref. [75]. Let $\bar{C}$ be the $3 \times N$-dimensional
stochastic vector ("master vector") consisting of the velocities of \( N \) particles

\[
\vec{C} = (\vec{v}_1, ..., \vec{v}_n).
\]

From now on we will only consider a spatially uniform case. Let us now define \( f_N(\vec{C}_1, t) \) be the probability density for the stochastic vector \( \vec{C} \) to have value \( \vec{C}_1 \) at time \( t \). We shall also introduce the function \( f_{N|N}(\vec{C}_1, t_1|\vec{C}_2, t_2) \) which is the conditional probability density for the stochastic vector \( \vec{C} \) to have value \( \vec{C}_2 \) at time \( t_2 \) given that it had value \( \vec{C}_1 \) at time \( t_1 \). The conditional density is defined by the identity:

\[
f_{2N}(\vec{C}_1, t_1; \vec{C}_2, t_2) = f_N(\vec{C}_1, t_1)f_{N|N}(\vec{C}_1, t_1|\vec{C}_2, t_2)
\]  \hspace{1cm} (2.1)

where \( f_{2N}(\vec{C}_1, t_1; \vec{C}_2, t_2) \) is the joint probability density for the stochastic vector to have a value \( \vec{C}_1 \) at time \( t_1 \) and the value \( \vec{C}_2 \) at time \( t_2 \). The joint probability densities are positive, normalized and can be reduced according to the formula:

\[
\int f_{2N}(\vec{C}_1, t_1; \vec{C}_2, t_2)d\vec{C}_1 = f_N(\vec{C}_2, t_2).
\]  \hspace{1cm} (2.2)

Combining (2.1) and (2.2), we obtain the following expression for the probability densities at different times:

\[
f_N(\vec{C}_2, t_2) = \int f_{2N}(\vec{C}_1, t_1)f_{N|N}(\vec{C}_1, t_1|\vec{C}_2, t_2)d\vec{C}_1.
\]  \hspace{1cm} (2.3)
Let us expand the conditional probability density $f_{N|N}(\vec{C}_1, t_1|\vec{C}_2, t_1 + \tau)$ in a Taylor series for small $\tau$ such that the normalization is preserved:

$$f_{N|N}(\vec{C}_1, t_1|\vec{C}_2, t_1 + \tau) = \delta(\vec{C}_1 - \vec{C}_2) - \tau \int W_{t_1}(\vec{C}_1, \vec{C})\delta(\vec{C}_1 - \vec{C}_2)d\vec{C} + \tau W_{t_1}(\vec{C}_1, \vec{C}_2)$$  

(2.4)

where $\delta(\vec{C}_1 - \vec{C}_2)$ is the $3 \times N$-dimensional Dirac’s delta function and $W_{t_1}(\vec{C}_1, \vec{C}_2)$ is the transition probability density per unit time that the system changes from the velocity state $\vec{C}_1$ to $\vec{C}_2$ in the time interval from $t_1$ to $t_1 + \tau$. Note, that we used the fact that $f_{N|N}(\vec{C}_1, t_1|\vec{C}_2, t_1) = \delta(\vec{C}_1 - \vec{C}_2)$.

Taking $t_2 = t_1 + d\tau$ in Eq. (2.3), we have:

$$f_N(\vec{C}_2, t_1 + \tau) = \int \{ f_N(\vec{C}_1, t_1)\delta(\vec{C}_1 - \vec{C}_2) - \tau \int W_{t_1}(\vec{C}_1, \vec{C})\delta(\vec{C}_1 - \vec{C}_2)d\vec{C} + \tau W_{t_1}(\vec{C}_1, \vec{C}_2) \} d\vec{C}_1$$  

(2.5)

We can simplify the right-hand side of the equation by applying the formula of the convolution with the delta function:

$$f_N(\vec{C}_2, t_1 + \tau) = f_N(\vec{C}_2, t_1) + \tau \int \{ W_{t_1}(\vec{C}_1, \vec{C}_2)f_N(\vec{C}_1, t_1) - W_{t_1}(\vec{C}_2, \vec{C}_1)f_N(\vec{C}_2, t_1) \} d\vec{C}_1.$$  

(2.6)

Rearranging terms in Eq. (2.6) and using the definition of the time derivative of the probability density:

$$\frac{\partial f_N(\vec{C}_2, t_1)}{\partial t} = \lim_{\tau \to 0} \frac{f_N(\vec{C}_2, t_1 + \tau) - f_N(\vec{C}_2, t_1)}{\tau}.$$  

(2.7)
we finally arrive at the following differential equation:

\[
\frac{\partial f_N(\vec{C}_2, t)}{\partial t} = \int \left\{ W(\vec{C}_1, \vec{C}_2)f_N(\vec{C}_1, t) - W(\vec{C}_2, \vec{C}_1)f_N(\vec{C}_2, t) \right\} d\vec{C}_1 \quad (2.8)
\]

known as *master equation*.

To obtain the N-particle kinetic master equation, two further assumptions are made. The first assumption, which is valid for dilute gases, is that only binary collisions are allowed for the transition of the system from one velocity state to another. That is the only possible transitions are when the velocities of molecules \(i\) and \(j\) are changing according to a collision mechanism involving the conservation of the momentum and energy. We will denote such transitions \(\vec{C} \rightarrow \vec{C}_{ij}^f\), where \(\vec{C}_{ij}^f = (v_{1i}, \ldots, v_{0i}^f, \ldots, v_{N}^f)\).

The second assumption is that the transition density is equal for the direct and reverse collisions, i. e. \(W(\vec{C}, \vec{C}_{ij}^f, t) = W(\vec{C}_{ij}^r, \vec{C}, t)\). This assumption is valid if the potential of the particle interaction is spherically symmetric. Taking these two assumptions into account, the master equations can be rewritten as:

\[
\frac{\partial f_N(\vec{C}, t)}{\partial t} = \frac{n}{N} \sum_{i<j} \int (f_N(\vec{C}_{ij}^f, t) - f_N(\vec{C}, t))w(v_{i}^f, v_{j}^f|v_{i}, v_{j})dv_{i}^f dv_{j}^f \quad (2.9)
\]

where \(w(v_{i}^f, v_{j}^f|v_{i}, v_{j})\) is the conditional probability density for a transition of a pair of particles from \((v_{i}, v_{j})\) to \((v_{i}^f, v_{j}^f)\).
The transition density and the differential collision cross-section are related by the equation:

\[ w(v_i^i, v_j^j | v_i^v, v_j^v) = \sigma(g_{ij}, \chi_{ij}) \delta(v_i^v + v_j^v - v_i^i - v_j^j) \delta((v_i^v - v_j^v)^2 - (v_i^i - v_j^j)^2) \]  \hspace{1cm} (2.10)

where \( \sigma \) is the differential collision cross-section, \( g_{ij} = |v_i^i - v_j^j| \) is the magnitude of the relative velocity and \( \chi_{ij} \) is the scattering angle. The two delta functions ensure the conservation of energy and momentum in the collision. The differential cross-section for binary elastic collision \( \sigma(g_{ij}, \chi_{ij}) \) is equal to \( |v_i^v - v_j^v| b_{ij} d\xi_{ij} \) where \( b_{ij} \) is the distance of closest approach of the undisturbed trajectories of particles \( i \) and \( j \), and \( \xi_{ij} \) is the angle between the collision plane and a fixed reference plane. Thus, the N-particle equation can be written as:

\[ \frac{\partial f_N(\vec{C}, t)}{\partial t} = \frac{n}{N} \sum_{i<j} \int_0^\infty \int_0^{2\pi} (f_N(\vec{C}_{ij}^v, t) - f_N(\vec{C}, t)) |v_i^i - v_j^j| b_{ij} d\theta_{ij} d\xi_{ij} \] \hspace{1cm} (2.11)

### 2.1.2 Connection between the master equation and the Boltzmann equation

For the probability density \( f_N(\vec{C}, t) \) where \( \vec{C} = (v_1^i, \ldots, v_N^i) \) we can introduce \( k \)-dimensional contractions

\[ f_k(v_1^i, \ldots, v_k^i) = \int f_N(\vec{C}, t) dv_{k+1} \ldots dv_N \] \hspace{1cm} (2.12)
By integration of the N-particle master kinetic equation with respect to $\vec{v}_2 \ldots \vec{v}_N$, we get [43]:

$$\frac{\partial f_1(\vec{v}_1, t)}{\partial t} = \frac{N - 1}{N} n \int \int (f_2(\vec{v}_1', \vec{v}_2') - f_2(\vec{v}_1', \vec{v}_2)) |\vec{v}_1' - \vec{v}_2'| b_{ij} d\xi_{ij} d\vec{v}_2$$

(2.13)

This equation transforms, as $N \to \infty$, into the Boltzmann equation

$$\frac{\partial f}{\partial t} = n \int \int (f(\vec{v}_1') f(\vec{v}_2') - f(\vec{v}_1') f(\vec{v}_2)) |\vec{v}_1' - \vec{v}_2'| b db de$$

if the molecular chaos property

$$f_2(\vec{v}_1', \vec{v}_2', t) = f_1(\vec{v}_1', t) f_1(\vec{v}_2', t)$$

(2.14)

holds. The molecular chaos property is a statement that the distributions of the two particles are independent. Note that even if the chaotic property holds, the N-particle master kinetic equation approximates the Boltzmann equation with an accuracy on the order of $O(1/N)$ where $N$ is the number of particles in the system.

### 2.2 DSMC numerical schemes for approximate solution of N-particle master kinetic equation

The N-particle master kinetic equation which is a non-linear integro-differential equation can be transformed to a Fredholm equation of the second kind. The latter has a solution in terms of the Neumann series provided that the convergence criteria is satisfied. In that case linear functionals of the N-particle distribution function ( such
as velocity, temperature and other macroparameters) can be calculated by the direct
simulation Monte Carlo method. The derivation in this section was first suggested by
Belotserkovsky and Yanitsky [12].

2.2.1 Construction of the direct simulation algorithm

If we introduce the collision frequency as

\[
\nu(\vec{C}) = \frac{n}{N} \sum_{i<j} \int w(\vec{v}_i^0, \vec{v}_j^0 | \vec{v}_i^0, \vec{v}_j^0) d\vec{v}_i^0 d\vec{v}_j^0 = \frac{n}{N} \sum_{i<j} g_{ij} \sigma_t(g_{ij})
\]  

(2.15)

where

\[
\sigma_t(g_{ij}) = \int_0^{2\pi} \int_0^\pi \sigma(g_{ij}, \chi_{ij}) \sin \chi_{ij} d\chi_{ij} d\varepsilon_{ij}
\]

is the total collision cross-section. We can now rewrite Eq. (2.9) as follows:

\[
\frac{\partial f_N(\vec{C}, t)}{\partial t} + \nu(\vec{C}) f_N(\vec{C}, t) = J_1
\]

(2.16)

where we denote

\[
J_1 = \frac{n}{N} \sum_{i<j} \int f_N(\vec{C}_{ij}, t) w(\vec{v}_i', \vec{v}_j' | \vec{v}_i, \vec{v}_j) d\vec{v}_i' d\vec{v}_j'.
\]

It is easy to check by direct substitution that the solution to Eq. (2.16) is given by:

\[
f_N(\vec{C}, t) = f_N(\vec{C}, 0) \exp\{-\nu(\vec{C})t\} + \int_0^t J_1 \exp\{-\nu(\vec{C})(t - t')\} dt'
\]

(2.17)
We can introduce the function \( \varphi(\bar{C}, t) = \nu(\bar{C}) f_N(\bar{C}, t) \) and multiplying Eq (2.17) through by \( \nu(\bar{C}) \), we get a Fredholm equation of the second kind for the function \( \varphi(\bar{C}, t) \):

\[
\varphi(\bar{C}, t) = \int_0^\infty \int K_1(\bar{C}' \to \bar{C}) K_2(t' \to t|\bar{C}) \varphi(\bar{C}', t') d\bar{C}' dt' + \varphi_0(\bar{C}, t) \tag{2.18}
\]

where

\[
\varphi_0(\bar{C}, t) = f_N(\bar{C}, 0) \nu(\bar{C}) \exp(-\nu(\bar{C})t)
\]

and we denoted

\[
K_1(\bar{C}' \to \bar{C}) = \frac{n}{N} \sum_{i<j} w(\bar{v}_i, \bar{v}_j|\bar{v}_i, \bar{v}_j) \nu^{-1}(\bar{C}) \prod_{m=1}^N \delta(\bar{v}_m - \bar{v}_m') \tag{2.19}
\]

\[
K_2(t' \to t|\bar{C}) = \theta(t - t') \nu(\bar{C}) \exp(-\nu(\bar{C})(t - t')). \tag{2.20}
\]

Here prime in Eq. (2.19) indicates that the factors with \( m = i \) and \( m = j \) are omitted.

The function \( \theta(t - t') = 1 \) if \( t > t' \) and \( \theta(t - t') = 0 \) otherwise. Note that \( K_2(t' \to t|\bar{C}) \) is the probability density for the random time between two collisions, and \( K_1(\bar{C}' \to \bar{C}) \) is the probability density of the transition from \( \bar{C}' \) to \( \bar{C} \).

In the succeeding analysis we will use the function \( \psi(\bar{C}, t) \) defined by the relation:

\[
\varphi(\bar{C}, t) = \int_0^\infty K_2(t' \to t|\bar{C}) \psi(\bar{C}, t') dt'. \tag{2.21}
\]

By direct substitution into Eq. (2.18) and taking into account that \( K_2 > 0 \), we find that

\[
\psi(\bar{C}, t) = \int_0^\infty \int K_2(t' \to t|\bar{C}') K_1(\bar{C}' \to \bar{C}) d\bar{C}' dt' + \delta(t) f_N(\bar{C}, 0). \tag{2.22}
\]
The kernel of this equation $K_{21} = K_{1} K_{2}$ satisfies the condition

$$
\int_{0}^{T} \int K_{21}(t', \bar{C}' \rightarrow t, \bar{C}) \, d\bar{C} \, dt < 1
$$

and, therefore, the Neumann series for Eq. (2.22) converges for arbitrary $T < \infty$ and the Monte Carlo method for calculating linear functionals of $\psi(\bar{C}, t)$ can be applied. Since

$$
K_{1}(\bar{C}'' \rightarrow \bar{C}) > 0, \quad K_{2}(t' \rightarrow t|\bar{C}) > 0
$$

and

$$
\int_{0}^{\infty} \int \delta(t)f_{N}(\bar{C}, t) \, d\bar{C} \, dt = 1, \quad \int K_{1}(\bar{C}'' \rightarrow \bar{C}) \, d\bar{C} = 1, \quad \int_{0}^{\infty} K_{2}(t' \rightarrow t|\bar{C}) \, dt = 1
$$

we can construct the direct simulation algorithm where the initial distribution of Markov chain is chosen as $\delta(t)f_{N}(\bar{C}, 0)$, the transition density from $(\bar{C}'', t')$ to $(\bar{C}, t)$ is chosen as $K_{12}(t', \bar{C}'' \rightarrow t, \bar{C})$.

The basic direct simulation algorithm can be constructed as follows:

1. The initial state $\bar{C}_{0}$ is sampled according to the probability density $f_{N}(\bar{C}, 0)$.

2. The collision frequency $\nu(\bar{C})$ is calculated according to Eq. (2.15).

3. The time between two collisions is sampled according to the density $K_{2}(t_{n} \rightarrow t_{n} + \tau), t_{n+1} = t_{n} + \tau$. The time $\tau$ between the two collisions is calculated by the formula

$$
\tau = -\nu^{-1}(\bar{C}_{n}) \ln(rand)
$$
where \( \text{rand} \) is the uniformly distributed on the interval \((0, 1)\). If \( t_{n+1} > T \) then the trajectory is terminated, next go to (1).

(4) The transition from state \( \tilde{C}_n \) to \( \tilde{C}_{n+1} \) is simulated according to the probability density \( K_1(\tilde{C}_n \rightarrow \tilde{C}_{n+1}) \), then go to (2). The simulation of the transition involves the sampling of \( \tilde{t} \) - the unit vector of direction of the relative velocity of the particles after the collision. To obtain the probability density \( p(\tilde{l}) \), one can integrate \( K_1(\tilde{C}' \rightarrow \tilde{C}) \) with respect to the variables \( \tilde{v}_1, \ldots, \tilde{v}_N \). This yields the following distribution:

\[
p(\tilde{l}) = \frac{\sum_{i<j} g_{ij} \sigma_t(g_{ij}) \sigma(g_{ij}, \tilde{l})}{\sum_{k<m} g_{km} \sigma_t(g_{km})}
\tag{2.23}
\]

The sampling from this distribution can be performed by the composition method. First, we choose random indices of the particles according to the discrete distribution

\[
\frac{g_{ij} \sigma_t(g_{ij})}{\sum_{k<m} g_{km} \sigma_t(g_{km})}.
\]

Next, the vector \( \tilde{l} \) is chosen according to the conditional probability density

\[
\sigma(g_{ij}, \tilde{l}) / \sigma_t(g_{ij})
\]

The computational cost of the algorithm makes its use impractical (the exact calculation of the collisional frequency \( \nu(\tilde{C}) \) involves \( O(N^2) \) operations) and the approximate schemes with cost linearly proportional to \( N \) were suggested.
2.2.2 Majorant frequency scheme

The following approximate numerical scheme for the direct simulation of the random process described by Eq. (2.22) was proposed by Ivanov and Rogasinsky [43]. The algorithm to model collisional relaxation during the time interval from 0 to $\Delta t$ is:

1. The initial state $\tilde{C}_0$ is chosen according to the probability density $f_N(\tilde{C}, 0)$ and $t_n = 0, n = 0$ are stored;

2. The time between two collisions is sampled as

$$\tau_m = -\nu_m^{-1} \ln(rand)$$

where $\nu_m = \frac{n(N-1)}{2} [g_{ij} \sigma_i (g_{ij})]_{\text{max}}$ is the majorant frequency, $\nu_m > \nu(\tilde{C})$. Time is changed $t_{n+1} = t_n + \tau_m$;

3. If $t_{n+1} > \Delta t$, then stop. If $t_{n+1} < \Delta t$, then a pair $(\tilde{v}_i, \tilde{v}_j)$ is uniformly chosen from the system of N particles and if

$$rand < \frac{g_{ij} \sigma_i (g_{ij})}{[g_{ij} \sigma_i (g_{ij})]_{\text{max}}}$$

then go to (4). Otherwise, go to (2).

4. The pair $(\tilde{v}_i, \tilde{v}_j)$ is chosen as collision pair and the new velocities $(\tilde{v}_0^i, \tilde{v}_0^j)$ are calculated similarly to step (4) in Section 4.1;

5. Go to (2).
The computational cost of the algorithm increases linearly with respect to the number of particles $N$. The majorant frequency scheme is more accurate than the widely used NTC scheme (described next) and it allows to model the collisional relaxation with smaller number of particles.

### 2.2.3 No Time Counter scheme

Another widely used approximate scheme of the DSMC method is the No Time Counter (NTC) scheme proposed by Bird [16]. In the NTC algorithm the collisions are not sampled from the exponential distribution but instead the average number of collisions is calculated for a given time step. Total number of pairs selected for possible collisions during a time step $\Delta t$ is equal to

$$\frac{n\bar{N}}{2}[g_{ij}\sigma(g_{ij})]_{max}\Delta t$$

where $\bar{N}$ is the average number of modeling particles during the calculation. Then, similarly to the majorant frequency scheme the collision of a pair is accepted if

$$\text{rand} < \frac{g_{ij}\sigma(g_{ij})}{[g_{ij}\sigma(g_{ij})]_{max}}.$$

The NTC scheme has the same computational complexity as the majorant frequency algorithm and predicts the same number of collisions on average. However, because in NTC scheme the time between collision is not sampled from the exponential distribution directly, the scheme requires a larger number of simulated particles in
each cell to be used to avoid a systematic error in the collision frequency. The majorant
frequency scheme has been used in all DSMC calculations presented in the next chapters.
Chapter 3

Gas Flow in Microthrusters

3.1 Background and motivation

MEMS-based micropropulsion concept is viewed by NASA’s mission planners as the enabling technology for spacecraft formation flying [30]. A spacecraft formation implies two or more miniature spacecraft that operate synchronously in a controlled spatial configuration. Miniature spacecraft are usually classified into three categories by the total mass [49]: microspacecraft (10-100 kg), nanospacecraft (1-10 kg), and, finally, picospacecraft (< 1 kg). Controlling a spacecraft formation will demand a wide range of propulsion maneuvers such as orbit raising, drag makeup, stationkeeping and deorbit. The minimum impulse bits on the order of mN-s may be required for microspacecraft missions.

New propulsion systems, therefore, are needed that are able to deliver precise impulse bits while meeting strict mass, size and power usage limitations. MEMS-based propulsion devices are being considered for such missions because of a number of their advantages: lightweight materials, high degree of integration between different components, ability to provide versatile thrust levels, and, finally, the potential to batch manufacture such devices. A MEMS-based propulsion system might consist of arrays of tiny rocket thrusters on a silicon chip with electronic circuitry that controls the firing. Currently,
various micropropulsion concepts are being considered, such as cold gas [74, 10], catalytic decomposition [35], vaporizing liquid [68] and mono- and bi-propellant [61] thrusters.

The utility of microthrusters to the new generation of space vehicles has been discussed by many researchers [45, 53, 67]. The advances in MEMS technology in the last decade have enabled the production of micron-sized rocket motors [36]. However, detailed theoretical and experimental study of the mechanics of the working fluid must be conducted before the utility of such micropropulsion devices can be assessed. One of the most important issues is an estimate of thrust performance at the small scale, possible with this new technology.

The dramatic change in the linear dimension affects both the mechanics of the working fluid and geometric design of micropropulsion devices. A typical flow in a cold-gas micron-sized thruster has low Reynolds number on the order of $10^2 - 10^3$ and viscous effects therefore will be much more significant than in conventional large nozzles (Reynolds number, typically, larger than $10^6$). Another consequence of the small linear scale for supersonic nozzle is the flow rarefaction resulting in the possibility of velocity slip and temperature jump at the gas solid surface interface. The surface area to volume ratio in micro devices is so high that the wall effects may dominate the fluid behavior inside the nozzle, thus requiring an accurate modeling of gas-surface interaction.

Often the geometric shape of a mechanical device is chosen to maximize the performance while minimizing the cost of manufacture. Since entirely different materials and manufacturing technology is used for MEMS, the geometric shape is different from that for large scale nozzles. The conventional rocket nozzles are almost always of an axisymmetric shape and often have a contoured section to direct the exhaust gas along
the axis. For the micro-fabrication of nozzle devices the technique is well developed for etching a simple-shaped device from a plane silicon wafer. Experimental measurements by Bayt et al [10] of mass flow and thrust levels of such flat contoured nozzles showed that for low Reynolds numbers $Re < 500$ nozzle performance is strongly affected by viscous losses and there is a considerable deviation from a two-dimensional Navier-Stokes solution because of the three-dimensional end-wall effects. Therefore, accurate numerical study of such flows requires a full three-dimensional simulation.

Several earlier studies [24, 21, 42, 40] presented computational results for axisymmetric cold gas nozzle flows at low Reynolds numbers. These studies employed the direct simulation Monte Carlo method. The work by Chung et al [24] was performed with the goal to make a comparison between numerical DSMC modeling and experimental data [76]. In the paper by Ivanov et al [42] both DSMC and continuum methods were used to simulate the axisymmetric and two-dimensional flow in a nozzle at low Reynolds numbers. The computational results presented here in Section 3.2 were the first application of the DSMC method to modeling three-dimensional microthrusters and have been published in Ref. [2].

Higher specific impulse values may be achieved when a high-temperature gas is generated [81]. Recently, a fabrication of a microturbine driven by a bi-propellant micro-combustor using MEMS technology has been reported [64]. In this work, temperatures on the order of 1000 K were obtained in a silicon-based hydrogen-air combustor of dimensions of several millimeters. This last result raises the possibility of fabricating new microrocket engines with high-temperature gases in the nozzle regions. The use of high-temperature gases in a rocket nozzle offers potentially higher specific impulses but the
effects of the temperature regime on performance of a microscale thruster has to be carefully studied due to higher viscous losses. The DSMC method has been employed by Zelesnik et al for the numerical study of cold and heated gas flows in axisymmetric nozzles of different axisymmetric nozzle shapes in Ref. [90]. The authors found that for higher gas temperatures the nozzle efficiency is below 50% due to heat losses in the viscous flow at $Re = 90$.

The above mentioned issues, important for microthruster performance in different temperature regimes, will be studied in this chapter. The outline of the chapter is as follows. Section 3.2 focuses on numerical study of viscous effects in cold gas micronozzle flow and a comparison of different geometric configurations, axisymmetric conical and flat three-dimensional, in terms of thrust performance and flow fields. The solutions of the Navier-Stokes equations are also obtained to elucidate the area of applicability of the continuum approach. A two-dimensional model of a micronozzle is also examined and compared with the full three-dimensional simulation in this section. In Section 3.3 the effects of the temperature regime on micronozzle performance are analyzed and the results of DSMC simulations are validated by comparison with experimental data. The results presented in this section were published in Ref. [6].

3.2 Simulation of cold gas micronozzle flows

3.2.1 Micronozzle configurations and flow conditions

Two different micronozzle configurations are considered in Section 3.2, axisymmetric and three-dimensional. The axisymmetric conical nozzle has an expansion angle
of 15 deg, throat diameter $D_t = 300 \, \mu m$, and an exit to throat area ratio of 100. A schematic of the three-dimensional (hereafter referred as flat) nozzle and axis notation are shown in Fig. 3.1. The throat width is equal to the axisymmetric nozzle throat diameter $D_t$, and the height $h = 300 \, \mu m$. The expansion angle is 15 deg, and the area ratio is 10. The flat nozzle dimensions are derived from the experimental study reported in Ref. [26, 74]. The flat nozzle has the same cross section in $X - Y$ symmetry plane as the axisymmetric nozzle, as well as the same nozzle length of 5.038 mm. The details on nozzle geometry and computational domain in $X - Y$ symmetry plane are given in Fig. 3.2.

For the two geometric nozzle configurations, the flow of molecular nitrogen was calculated at a stagnation pressure $p_c = 10 \, kPa$ and stagnation temperature $T_c = 300 \, K$. Stagnation and critical conditions for a sonic flow at the throat are given in Table 3.1. The Knudsen number at the throat for both nozzles is $5 \times 10^{-3}$ and the corresponding Reynolds number based on the throat half-width is 200. The temperature at the nozzle wall is assumed to be constant and equal to the stagnation temperature at the chamber.

3.2.2 Continuum method

A continuum model was used to describe the gas flow in the axisymmetric and three-dimensional nozzles. The numerical solution of the Navier-Stokes equations for viscous fluid flow was obtained with a finite-volume spatial discretization on a structured three-dimensional grid implemented in the General Aerodynamic Simulation Program (GASP [31]).
Molecular nitrogen was considered a perfect gas and the Sutherland model [86] was used for the approximation of temperature dependence of the gas viscosity. Viscous derivative terms in the momentum and energy conservation equations are computed with second-order accuracy on the interior and gas-solid interface cells. The third-order upwind-biased scheme is applied for spatial reconstruction of volume properties on the cell boundaries. To obtain a steady state solution two factor approximate factorization is used for time stepping.

As was shown by Ivanov et al [42], an extrapolation boundary condition at the exit of a nozzle can sufficiently decrease the accuracy of the performance prediction at low Reynolds numbers. Therefore, an exterior region of nozzle was also included in the computational domain. Two-zone grids resolving gradients near wall boundaries and along the axis are used in the computations. A grid convergence study showed that the solution is grid independent for grid dimensions $200 \times 40$ (zone 1) and $100 \times 60$ (zone 2) and larger for the axisymmetric and 2D case and $200 \times 40 \times 20$ (zone 1) and $100 \times 60 \times 20$ (zone 2) for the 3D case. The GASP MPI capabilities allow iterations in different regions of the computational domain to be performed in parallel. Using this option on a two processor SGI Octane the total computational time for the axisymmetric case with the grid $200 \times 40$ and $100 \times 60$ is about 8 hours and about 50 hours for the 3D case.

A no-slip boundary condition is used in these computations to model gas-surface interaction at a fixed wall temperature. The temperature of the wall is set to the stagnation temperature at the chamber. The inlet conditions are obtained from ideal nozzle theory based on stagnation gas properties and an inlet area ratio. For the axisymmetric case both subsonic and critical inlet conditions are considered. For the subsonic inlet
conditions the boundary layer is thin at the nozzle throat. This is illustrated in Fig. 3.3 where the velocity component in X direction along the nozzle axis is shown. The difference between solutions for these two types of inlet conditions is therefore small. The comparison of Mach number fields is given in Fig. 3.4. There is a very small difference in the results. For a quantitative comparison, the X-component velocity distribution along the nozzle axis is given in Fig. 3.5. The nozzle performance characteristics of the axisymmetric nozzle are also very close (see Table 3.2). The constant critical throat condition is therefore used to as the boundary conditions for the axisymmetric and three-dimensional solutions calculated with the Navier-Stokes and DSMC methods.

3.2.3 DSMC method

The DSMC calculations presented in this chapter were obtained using a DSMC-based software SMILE (Statistical Modeling In a Low-density Environment) [41]. The majorant frequency scheme of the DSMC method is utilized to model collisions between molecules. The intermolecular potential is assumed to be the variable soft sphere model [54]. The Larsen-Borgnakke model [20] with temperature-dependent $Z_r$ and $Z_v$ and discrete rotational and vibrational energies is used for the energy exchange between translational and internal modes.

Under flow and geometry conditions examined in this section, the wall can be expected to significantly affect the gas flow. One of the most widely used gas-surface interaction models, the Maxwell model, assumes that a fraction $(1 - \alpha_r)$ of incident particles is reflected specularly while the remaining fraction $\alpha_r$ experiences a diffuse reflection that means particle velocities are distributed according to the Maxwellian
distribution with the surface temperature. This parameter $\alpha_\tau$ is equal to tangential momentum accommodation coefficient:

$$\alpha_\tau = \frac{P_{i\tau} - P_{r\tau}}{P_{i\tau}},$$

where $P_\tau$ is the tangential momentum, and indices $i, r$ refer to incident and reflected particles. Experimental data [8] for silicon interacting with nitrogen flow suggests the accommodation coefficient $\alpha_\tau = 0.8$. The Maxwell model with different $\alpha_\tau$ between 0 and 1 and the surface temperature $T_w = 300$ K is used in these DSMC computations.

Convergence studies of the DSMC solution in terms of the number of particles was conducted for the three-dimensional micronozzle. The translational temperature and velocity component $U_x$ profiles along the nozzle centerline are plotted in Fig. 3.6 and 3.7 for different number of simulated particles in the computational domain: $N = 1.3 \cdot 10^6$, $5 \cdot 10^6$, $10^7$, $2 \cdot 10^7$. The simulations show that there is a significant dependence of the results on $N$ in the region of high density. As it is seen from the profiles, the DSMC solution for a smaller number of particles is shifted. The converged DSMC solution is obtained for 10 million simulated particles. The three-dimensional DSMC calculations have been performed using 16 processor 250 MHz Origin 2000 with the total computing time of about one hundred hours.

3.2.4 Axisymmetric conical nozzle

Let us consider first the flow in an axisymmetric conical micronozzle that was studied with the continuum and DSMC methods. A comparison of density fields obtained
by the two techniques is given in Fig. 3.8. The density is normalized by its value at the nozzle throat.

The flowfields for the axisymmetric micronozzle are those typical for cold gas thrusters. The gas experiences about two orders of magnitude decrease in density along the nozzle axis (see Fig. 3.9). In the radial direction the density decreases near the wall because the temperature of the wall is higher than that of gas. Contours of the velocity component in the axial direction obtained by both models are plotted in Fig. 3.10. It is seen that the numerical solution of Navier-Stokes equations agrees well with the DSMC results inside the nozzle and at the core flow outside the nozzle. There is a significant difference between the two solutions only in the region of the nozzle lip. The reason for that is a rapid expansion of gas and a high flow rarefaction that is difficult to capture by continuum methods.

Velocity contours qualitatively illustrate how the thickness of the boundary layer grows downstream from the nozzle throat. To study the boundary layer growth in more detail, the distribution of the X-component of velocity at the nozzle exit is given in Fig. 3.11. The velocity gradient is large close to the axis and the boundary layer occupies most of the exit area. The difference between the velocities at the wall for the two approaches is due to the difference in their boundary conditions. However, a comparison of velocity profiles along the nozzle axis presented in Fig. 3.12 shows a small difference between the two solutions.

Translational temperature contours are shown in Fig. 3.13 for two different approaches. The agreement is satisfactory inside the nozzle except in the vicinity of the lip where the impact of flow rarefaction is again significant. The GASP solver assumes there
is an equilibrium between translational and internal modes. While the vibrational mode is essentially frozen at the low temperatures under consideration, and vibrational excitation is not an important factor, the rotational temperature may be significantly different from the translational one. Figure 3.14 shows the DSMC rotational and translational temperature profiles along the nozzle axis compared with those obtained by GASP. Differences between the translational and rotational temperatures beyond the nozzle exit can be observed. The difference between the translational temperatures obtained by the continuum and kinetic approaches caused both by the rarefaction and wall effects increases starting from 1 mm downstream from the nozzle exit.

3.2.5 Comparison of 2D and 3D models

A two-dimensional model can be used to describe the flow in a nozzle of a flat geometric configuration if the influence of the end-walls is negligible. However, as it is shown in the previous section for an axisymmetric flow, the entire area of the nozzle exit is affected by the wall boundary layer. In the flat nozzle case with the same flow conditions at the throat an even larger impact of viscous effects can be anticipated because of a greater surface area to volume ratio. A full three-dimensional modeling is therefore required to simulate the gas flow and accurately predict the performance characteristics of a three-dimensional high aspect ratio micronozzle.

To examine a possible contribution of the third dimension at given conditions, the modeling of 2D and 3D flows in a flat micronozzle was conducted using the continuum and kinetic approaches. The density contours are shown in Fig. 3.15 for both the 2D and 3D flow models. Whereas the density decreases gradually in the 2D case, in the 3D
nozzle the flow experiences two successive expansions, at the nozzle throat and the exit. This is due to the contribution of two different processes, the viscous dissipation and the flow expansion. This is also seen in Fig. 3.16 where the pressure fields are shown for the two flow models under consideration. Again, there is a significant difference between the two cases. The pressure is higher inside the nozzle for the 3D case due to the wall effect, with the core flow values approximately seven times larger. In the expansion region, downstream of the nozzle exit, the pressure is lower for the 3D case (the flow expands in three dimensions in this case).

A comparison of velocity fields for the two cases is given in Fig. 3.17. As expected, the 2D model predicts the values of the velocity component in the $X$-direction to be larger inside the nozzle. For the 3D case, the velocity increases at first 1 mm downstream from the throat (the flow expansion dominates there), and then slightly decreases towards the exit since the wall effects become more important. The velocity has a local maximum of 450 m/s at $\sim 1$ mm from the throat. The flow expands rapidly after the exit, and the velocity at 2 mm from the exit is even greater than in the 2D case.

The translational temperature fields are also qualitatively different for the two cases (see Figure 3.18). The temperature decreases downstream in the direction of the nozzle axis and increases at the wall (the gas is cooler than the surface) for the 2D case. There is a local minimum of temperature at 1 mm from the throat in the 3D flow, and temperature values are generally higher inside the nozzle and lower downstream from the exit plane for this case. The influence of the end-walls is therefore very important for the height to width ratio considered. For larger ratios, a smaller effect is expected,
and likewise there should be a smaller difference between 2D and 3D models since the
difference in the expansion process would be reduced.

The difference in the expansion process is illustrated in Fig. 3.19 where the molec-
ular local mean free path is plotted. The mean free path decreases gradually inside the
3D nozzle. It changes by a factor of three from the throat to the exit. For the 2D case
it drops more rapidly, and there is also a strong mean free path reduction across the
nozzle. Note, the local characteristic length for the 3D case is equal to the nozzle height
$h=300 \mu m$. The local Knudsen number at the exit plane is therefore about 0.1 which
falls into a regime where the continuum model fails.

3.2.6 Wall effects in axisymmetric and 3D nozzles

The surface area to volume ratio represents the relative impact of surface and
volume forces on the flow. For the MEMS scale devices the ratio is very high and the wall
effects can dominate the expansion process in the flow through a micronozzle. To choose
reasonable geometric parameters ensuring an expanding flow through a micronozzle, an
estimate of the boundary layer thickness at the exit has to be made, aimed at a decreasing
its thickness. A possible approach to nozzle design could be to utilize a flow over a plate
for an assessment of the boundary layer thickness growth. In a nozzle, though, the
boundary layer thickness grows much more rapidly than that over over a plate due to
the gas expansion. A full simulation is therefore required to examine the boundary layer
grows for a specified nozzle geometry.

To understand how the boundary layer grows in a 3D nozzle under chosen condi-
tions, Fig. 3.20 shows the translational temperature contours at different cross sections
perpendicular to the nozzle axis. The viscous layer is developed very rapidly, and at a
distance of several throat widths, it occupies the entire cross-sectional area. There is
therefore no inviscid core in the gas flow inside the nozzle at the Reynolds number and
aspect ratio modeled in this work.

The wall effects and flow expansion strongly impact the flow in a 3D nozzle
as compared to that in an axisymmetric nozzle. Figure 3.21 shows the translational
temperature profiles along the nozzle axis for the 3D and axisymmetric cases. After an
initial decrease at the first 1 mm due to the gas expansion, the temperature increases in
the 3D nozzle. Such an increase is caused by the viscous dissipation of the flow kinetic
energy of the flow due to the shear on the walls. Beyond the nozzle exit where gas
experiences a free expansion into a vacuum the velocities and temperatures coincide for
the two cases, since the mass flow rates are equal.

A qualitative difference between the two solutions shown for the temperature
profiles is also observed for the velocity fields. The profiles of the velocity in the X
direction are presented in Fig. 3.22. The velocity increases monotonously downstream
from the nozzle exit in the 2D case, while in the 3D flow there is a velocity minimum
located at $X = 0.004 \text{ m}$. The increase of temperature (see Fig. 3.21) and decrease in
velocity in the three-dimensional nozzle is a consequence of the shear on the walls. For
a hypersonic nozzle flow expanding into vacuum one would expect the extremum to be
at the exit plane. However, the extremum is located upstream of the nozzle exit because
of the subsonic region at the walls. These results show that impact of the walls is very
pronounced in the 3D case.
The model used to simulate the gas-surface interaction is therefore important. Since all results presented above were obtained using the tangential momentum accommodation coefficient $\alpha_T = 1$, different values of $\alpha_T$ were also used to examine the possible influence of the surface model. The DSMC computations were performed both for the axisymmetric and three-dimensional nozzles for different values of $\alpha_T$.

Translational temperature profiles along the nozzle axis for different $\alpha_T$ are shown in Fig. 3.23. The temperature increases with $\alpha_T$. There is a qualitative difference between the solution for $\alpha_T = 0$ (ideally smooth adiabatic surface) and any non-zero $\alpha_T$ for which the profile has a kink after the nozzle exit. There is also a visible difference between $\alpha_T = 0$, $\alpha_T = 0.3$, and $\alpha_T = 0.5$ profiles. Experimental work by Arkilic [9] suggests that a value of $\alpha_T = 0.8$ is recommended for a nitrogen flow in a silicon microchannel. The result for an axisymmetric nozzle flow with $\alpha_T = 0.8$ is very close to the solution with $\alpha_T = 1$.

A greater influence of the gas surface interaction model on the solution can be anticipated in 3D case where, as it was shown above, the wall effects dominate the flow inside the nozzle. Two cases were considered, $\alpha_d = 0.8$ and $\alpha_d = 1$. The DSMC results for these two cases are shown in Fig. 3.24 where the translational temperature contours are plotted. There is a subtle difference in the core flow, but generally the temperatures are very close for these two cases. The difference between the density fields is also small (see Fig. 3.25). The specific impulse for these two cases was calculated and the difference was found to be less than one percent. Note, a similar weak dependence of thrust performance for non-zero accommodation coefficients was shown for micro-resistojets in a recent paper [51].
3.2.7 Cold gas nozzle performance

The calculated thrust levels and specific impulses for different micronozzle configurations are summarized in Table 3.3. For the cases considered, the GASP solution slightly (several percent) overpredicts the thrust values obtained by the DSMC method. Comparing axisymmetric and three-dimensional results, the thrust as well as the specific impulse are lower for a flat micronozzle. The wall effects in the 3D case also cause an about 20 percent reduction in thrust as compared to the 2D model. Note that the 2D model gives the highest thrust values for the three cases under consideration. The specific impulse is also highest for the 2D model (5 percent greater than for the axisymmetric nozzle and 20 percent greater than the three-dimensional nozzle).

The total impulse flux at different locations downstream of the throat of the 3D nozzle obtained by the DSMC method is plotted in Fig. 3.26. There is an undesirable reduction in thrust in the second half of the nozzle caused by the viscous losses. The way to increase the performance would be to make the micronozzle shorter or to increase its height.

3.3 High-temperature micronozzle flows

3.3.1 Comparison with experimental data

A comparison with available experimental data [69] has been performed to validate the DSMC models and algorithms. Results of the comparison are presented in this section. Measurements of specific impulse efficiency of an axisymmetric nozzle for a range of low Reynolds numbers have been reported in Ref. [69]. In that work, centimeter
scale nozzles have been tested over a range of chamber pressure values in such a way that high enough thrust levels are produced to be measured with precision. The gas temperature in the static chamber was elevated by a resistance heating element, and nitrogen gas expansion through nozzles of different geometries was studied. Results of the measurements were also compared in Ref. [69] with the compressible boundary layer (BL) approximation calculated according to the Cohen-Reshotko procedure [25]. Note that a zero heat transfer to the wall was assumed in the approximation of Ref. [69].

To compare with the experimental data, nitrogen flow at a stagnation temperature of $T_0 = 1,033 \, K$ through an axisymmetric conical nozzle with an expansion angle of 20 deg and an area ratio of 100 is modeled for different Reynolds numbers, $Re = 178, 306, 409$. The full accommodation of tangential momentum ($\alpha_d = 1$) and different energy surface models has been used in the DSMC calculations. The calculated translational temperature contours for $Re = 178$ are plotted in Fig. 3.27 for three cases: adiabatic conditions ($\alpha_E = 0$) and two different wall temperatures $T_w = 300$ and 500 K ($\alpha_E = 1$). The calculated temperature field solution is sensitive to the type of wall conditions in the latter two cases and the difference in translational temperature between adiabatic conditions and constant $T_w$ at the nozzle exit is about 25%.

The measured and calculated axisymmetric nozzle efficiencies are plotted in Fig. 3.28. While the calculated thrust increases a factor of two with an increase in the Reynolds number from 200 to 400, the calculated efficiency growth is strongly hampered by viscous losses. The total efficiency rise in the experiment is only 5%; and there is a good agreement with the computational results shown in Table 3.5. The boundary layer approximation used in Ref. [69] predicts a decrease in nozzle efficiency when the Reynolds
number decreases. But the efficiency is overestimated due to the fact that heat transfer to the wall has been neglected in this approximation. Note, the wall temperature was not given in Ref. [69] but is expected to be higher than room temperature, 300 K, and significantly lower than the stagnation temperature of 1,033 K. That is why the DSMC computations were performed for constant wall temperatures of 300 and 500 K, and an adiabatic wall ($\alpha_d = 1, \alpha_E = 0$). The DSMC results are in good agreement with the experimental data for the case of $T_w = 500$ K, for which the calculated points fall within 0.5% from the experimental ones. They are somewhat lower (within 2.5 %) for a wall temperature of 300 K and significantly overestimate the data for the assumption of an adiabatic wall. The prediction of nozzle performance is therefore sensitive to the choice of wall temperature and energy accommodation coefficient in the surface model. The influence of the energy and momentum accommodation coefficients on the nozzle flow for different temperature regimes is further analyzed in the next section.

3.3.2 Effects of the accommodation coefficient and temperature regime

A study of influence of the surface energy and momentum accommodation coefficients on the simulation results for both cold and heated nozzle flows is carried out in this section. Molecular nitrogen expanding through a conical micronozzle at a low Reynolds number is used for this purpose. The expansion half-angle is 15 deg, the throat radius is 150 $\mu$m and the area ratio is 100. Three sets of chamber conditions were chosen to study low and high temperature flows at the same Reynolds number (they will be referred to as cold, heated, and high-temperature flows). Throat conditions for these sets are calculated from chamber conditions for an isentropic expansion and are listed
in Table 3.6. In all three cases, the Knudsen number based on the nozzle diameter is $2.77 \times 10^{-3}$, and the Reynolds number is 410.5.

For these flow conditions, different values of accommodation coefficients in the Maxwell gas-surface interaction model were used (see Table 3.4). Case 1 corresponds to an ideally smooth surface with no momentum and energy transfer between the gas flow and the wall. The second case is the diffuse reflection with an adiabatic wall, i.e. an average tangential momentum of reflected particles is equal to zero and no energy transfer occurs during particle-surface collisions. The last case implies both momentum and energy transfer with the wall at a constant temperature of 300 K.

For these flow conditions, different values of accommodation coefficients in the Maxwell gas-surface interaction model were used (see Table 3.4). Case 1 corresponds to an ideally smooth surface with no momentum and energy transfer between the gas flow and the wall. The second case is the diffuse reflection with an adiabatic wall, i.e. an average tangential momentum of reflected particles is equal to zero and no energy transfer occurs during particle-surface collisions. The last case implies both momentum and energy transfer with the wall at a constant temperature of 300 K.

**Cold gas flow**

Consider first a cold gas flow through the nozzle with Set 1 throat conditions. The calculated translational temperature contours are plotted in Fig. 3.29 for three types of gas-surface interaction. In Case 1 where the tangential momentum of molecules collided with the wall is conserved, there is no surface friction and no heat transfer occurs to the wall. No boundary layer develops at the wall in this case. In Cases 2 and 3 the translational temperature in the boundary layer near the wall is higher than that in the
core flow because of viscous dissipation of the flow kinetic energy. The translational temperature profiles along the nozzle centerline are plotted in Fig. 3.30. The difference between the results for an adiabatic wall (Case 2) and a constant wall temperature (Case 3) is small because the wall temperature is equal to the stagnation temperature of the flow. There is a local maximum of temperature observed at the nozzle exit for the last two cases, which is connected with the significant growth of the boundary layer.

Table 3.7 gives calculated nozzle performance characteristics for Set 1. The specific impulse in Case 1 is very close to the ideal nozzle theory prediction. In Cases 2 and 3 the efficiency of the nozzle is about 20% lower. The difference in $I_{sp}$ between the results for the adiabatic wall and a constant wall temperature is small because, again, the wall temperature is equal to the stagnation temperature of the flow.

**Heated flow**

The structure of a heated flow for different surface models is illustrated in Fig. 3.31. Comparison with Fig. 3.29 shows that for a heated flow the flowfield structure is more sensitive to the gas-surface model than for a cold gas. It is seen that the temperature near the wall is maximum for Case 2. This is due to the viscous dissipation of kinetic energy on the wall where the flow velocity drops and temperature increases. In this case there is no heat transfer to the wall and the temperature is higher than in Case 3, where it decreases due to heat losses. The influence of the heat losses in Case 3 is more evident in the translational temperature profiles along the nozzle axis, shown in Fig. 3.32. In contrast to the cold gas flow (Fig. 3.30), the calculated translational temperature for the heated flow depends on the energy accommodation coefficient $\alpha_E$. 
The calculated thrust performance of the heated nozzle flow is given in the Table 3.7 for different accommodation parameters. The thrust is maximum in Case 1 because no heat and momentum losses occur at the wall. In Case 2 the efficiency is 17.3% lower than in the ideal case due to the surface friction. In Case 3 thrust performance is lower by 27% due to the friction and heat transfer losses. The specific impulse for the heated flow is higher than that for the cold gas flow, but the efficiency is much lower due to additional heat transfer losses.

**High-temperature flow**

The nozzle flow with the stagnation temperature of 2,000 K was calculated using different surface models. The translational temperature contours (Fig. 3.33) show a significant difference in the flowfields calculated with different surface models. Calculated temperature profiles along the nozzle centerline are plotted in Fig. 3.34. In the high-temperature case, the difference between the adiabatic wall model and a constant wall temperature (Case 3) increases.

Calculated performance characteristics are listed in Table 3.7. When the baseline Case 3 surface model is used, the specific impulse in the high-temperature gas flow is about two times bigger than that for the cold gas.

Figure 3.35 shows a plot of thrust versus axial station for all three sets of throat conditions for a constant wall temperature model. The axial distance is normalized by the throat radius and the thrust is normalized by its value at the throat. It is seen that in the cold gas case the thrust is increased a maximum of 22% whereas in the heated and high-temperature cases the maximum value of thrust is 10% and 7.5% larger than
that at the throat. Therefore, a shorter nozzle (or a simple sonic nozzle) would be more practical for a high stagnation temperature flow at a Reynolds number of 200.

It is concluded from these results that the choice of the gas-surface interaction model is important for an accurate numerical prediction of the nozzle performance at low Reynolds numbers. The specific impulse of the high temperature thruster is as expected higher than that of a cold gas thruster. However, heat transfer losses are very significant and need to be considered. The performance of high-temperature nozzles operating at low Reynolds numbers can be optimized by geometric design with a shorter divergent section.

3.3.3 Heated flow in a 3D nozzle

In this section, a heated flow in a three-dimensional nozzle from Section 3.2 is considered. The stagnation temperature is $1,000 K$ and the throat-based Reynolds number is the same at 205. The diffuse model with a constant wall temperature of $300 K$ is assumed.

The calculated number density contours in the $X - Y$ symmetry plane for a cold and heated flow are shown in Fig. 3.36. The flow structure is different for the two temperature regimes, since in the cold gas case the wall temperature is equal to the stagnation temperature, whereas in the heated gas case the wall temperature is lower. In both cases the flow is dominated by the surface. It is illustrated by the profile of velocity in $X$ direction along the nozzle centerline shown in Fig. 3.37. The velocity in both cases has a maximum at approximately one fourth of the nozzle length and after that it drops due to viscous dissipation of the flow kinetic energy. Note that the decrease
of the velocity at the centerline due to wall effects shows that the boundary layer occupies the whole cross-sectional area of the nozzle. The calculated specific impulse is 56.6 (see Table 3.3) and 61.0 sec for the cold and heated cases, respectively. The increase of the specific impulse is considerably less than that in the axisymmetric flow due to larger surface area to volume ratio.

3.3.4 Hydrogen-air propellant flow in a conical nozzle

The performance of an axisymmetric nozzle has been calculated for the exhaust gases of the microcombustor [64] which uses hydrogen and air. The microcombustor produced temperatures in excess of 1,600 K. To simulate the flow in an axisymmetric nozzle for the combustion products generated by a microcombustor, the modeling has been performed for different pressures $p_0 = 0.1, 0.5$ and 1 atm. A stagnation temperature equal to the adiabatic flame temperature will be assumed in the modeling. The product composition was calculated for an equilibrium combustion at a constant pressure and for the stoichiometric fuel-to-oxidizer ratio. Only the major hydrogen-air combustion products, $\text{N}_2$, $\text{H}_2\text{O}$, and $\text{H}_2$, were assumed to be present in the nozzle flow. The stagnation temperature and species mole fractions are given in Table 3.8. The flow through an axisymmetric nozzle with a throat radius of 1 mm and an area ratio of 100 is simulated, for the Reynolds numbers based on the throat diameter of 208, 1,000, and 1,976.

Figure 3.38 shows the calculated translational temperature normalized by its value at the throat for stagnation pressures of 0.1 and 0.5 atm. The temperature fields are similar for the first third of the nozzle. Further downstream, the difference is more pronounced, with the temperature being higher for the less dense case.
The calculated specific impulse at different axial stations is plotted in Fig. 3.39 for stagnation pressures $p_0=0.1$, 0.5 and 1.0 atm. For lower pressures the peak value of $I_{sp}$ is closer to nozzle throat.

Let us now consider the impact of the molecular internal degrees of freedom. For cold gas thruster conditions, rotational relaxation is the dominant internal energy transfer process. In a high-temperature polyatomic gas, though, the excitation of molecular vibrations may become important. To study the possible effect of vibrational-translational (VT) energy transfer, the temperature-dependent and constant values of relaxation numbers $Z_r$ ($Z_r = 5$) and $Z_v$ in the Larsen-Borgnakke model have been used in the calculations.

Modeling of temperature-dependent water vibrational relaxation was performed using Eq. (3) of Ref. [66] assuming water molecules have three vibrational modes with one characteristic temperature of 2258 K. The corresponding $Z_v(T)$ changes from $10^4$ at 2,000 K to $10^6$ at 600 K. The vibrational relaxation of H$_2$O is not well known but is expected to be higher than the slow rates of the temperature-dependent model. Therefore, the constant values of $Z_v = 1$ and 100 were used that correspond to very fast and moderate rates of VT transfer.

Figure 3.40 shows the calculated specific impulse for $p_0 = 1$ atm and different relaxation numbers. It is seen that there is a significant difference (about 5 %) in the results depending on the vibrational energy relaxation number. As expected a faster VT relaxation increases the transfer of flow internal energy into kinetic energy and thus increases the nozzle performance.
3.4 Summary

A numerical study of different geometric configurations of micronozzles – axisymmetric and three-dimensional, has been conducted for a low throat Reynolds number of 200 using the DSMC method and the solution of Navier-Stokes equations.

The subsonic inflow conditions as well as critical throat conditions were considered in continuum computations. The results of the computations were shown to be insensitive to the type of inflow conditions both for thrust performance and flow fields.

The DSMC simulation of a three-dimensional flow at a Reynolds number of 200 is very computationally intensive. It is necessary to take at least 10 million simulated particles to obtain a particle-independent solution.

The DSMC and Navier-Stokes solutions are in a satisfactory agreement for the flow inside the nozzle. There is a significant difference between them in the region near the lip where the flow expands rapidly. The use of an external zone in the continuum approach, that starts at the nozzle exit and expands downstream, allows one to eliminate the possible impact of the extrapolation outflow boundary condition at the nozzle exit. This results in thrust values that are in agreement with those obtained by the DSMC method.

The effect of the wall accommodation coefficient was investigated by the DSMC method. The flow was found to be weakly dependent on the tangential momentum accommodation coefficient when it changes from 0.8 to 1 both for axisymmetric and three-dimensional cases. The flow changes significantly for accommodation coefficients smaller than 0.5.
The impact of wall effects on thrust level was examined for axisymmetric and three-dimensional micronozzles. A two-dimensional model was also used for the comparison. The flow in a flat nozzle has a three-dimensional structure and is strongly influenced by the end-walls. That causes a significant (about 20 percent) reduction in thrust as compared to the two-dimensional model and an axisymmetric nozzle. Attempts to predict the performance characteristics of a 3D microthruster using a 2D model may therefore result in significant design errors.

The influence of the gas-surface interaction model was examined for axisymmetric nozzle through variations of energy and momentum accommodation coefficients in three temperature regimes. The selection of the surface model is shown to be more important for a high-temperature nozzle flow at a low Reynolds number of 200. In a high-temperature flow the difference in $I_{sp}$ due to variations of the energy accommodation coefficient is 18 %. In a cold gas flow, where the stagnation temperature is close to the wall temperature, the variation of energy accommodation coefficient does not significantly change the nozzle efficiency. The choice of momentum accommodation coefficient is important for all temperature regimes. Its impact on thruster efficiency is slightly dependent on the stagnation temperature, at a fixed Reynolds number. The specific impulse was shown to be two times larger for the stagnation temperature of 2,000 K, than for the 300 K case, and the efficiency is only 10 % smaller for the higher temperature case.

The results of the thrust efficiency calculations using DSMC method were compared with reported experimental data for a heated nitrogen flow (stagnation temperature of 1,033 K). The DSMC results are in good agreement with the experimental data.
if a wall temperature of $T_w = 500$ K is assumed. The numerical results for the specific impulse efficiency were found to agree with the experimental data for Reynolds numbers of 178, 306 and 409 within 0.5% agreement. However for a lower wall temperature of 300 K and an adiabatic wall model, the simulation significantly overestimates the data. Therefore, such flow is strongly non-adiabatic and a general capability to model coupled, time-dependent fluid and thermal behavior in micro-combustion devices is required.

<table>
<thead>
<tr>
<th>Test gas</th>
<th>$N_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stagnation temperature $T_c$</td>
<td>300 K</td>
</tr>
<tr>
<td>Stagnation pressure $p_c$</td>
<td>10 kPa</td>
</tr>
<tr>
<td>Critical pressure $p_t$</td>
<td>5.2 kPa</td>
</tr>
<tr>
<td>Critical temperature $T_t$</td>
<td>250 K</td>
</tr>
<tr>
<td>Wall temperature $T_w$</td>
<td>300 K</td>
</tr>
</tbody>
</table>
Table 3.2. Nozzle performance characteristics for GASP solution with different inlet conditions for an axisymmetric nozzle.

<table>
<thead>
<tr>
<th>Condition</th>
<th>Thrust, mN</th>
<th>$I_{sp}$, sec</th>
</tr>
</thead>
<tbody>
<tr>
<td>subsonic inlet</td>
<td>1.08</td>
<td>66.06</td>
</tr>
<tr>
<td>uniform throat</td>
<td>1.07</td>
<td>65.62</td>
</tr>
</tbody>
</table>

Table 3.3. Nozzle performance characteristics.

<table>
<thead>
<tr>
<th>CASE</th>
<th>Thrust, mN</th>
<th>$I_{sp}$, sec</th>
</tr>
</thead>
<tbody>
<tr>
<td>AS GASP</td>
<td>1.07</td>
<td>65.62</td>
</tr>
<tr>
<td>AS SMILE</td>
<td>1.03</td>
<td>65.50</td>
</tr>
<tr>
<td>2D GASP</td>
<td>1.17</td>
<td>69.45</td>
</tr>
<tr>
<td>2D SMILE</td>
<td>1.10</td>
<td>68.74</td>
</tr>
<tr>
<td>3D SMILE</td>
<td>0.93</td>
<td>56.61</td>
</tr>
</tbody>
</table>
Fig. 3.1. Schematic of flat micronozzle.

Fig. 3.2. Nozzle geometry and computational domain in $X - Y$ plane.
Table 3.4. Summary of cases considered in Section 3.3

<table>
<thead>
<tr>
<th>Flow Conditions</th>
<th>Designation</th>
</tr>
</thead>
</table>

**Comparison with Experiment**

*Axisymmetric conical nozzle*

| A=100, α = 20°, N₂ | T₀ = 1,000 K | different Re numbers |

**Effect of Temperature**

*Axisymmetric conical nozzle*

| A=100, α = 15°, N₂ | T₀ = 300 K | “cold” gas, set 1 |
| T₀ = 1,000 K | “heated” gas, set 2 |
| T₀ = 2,000 K | “high-temperature”, set 3 |

*3D, high-aspect ratio*

| T₀ = 300 K |

**Surface Models**

| αₜ = 0, αₑ = 0 | case 1, specular reflection |
| αₜ = 1, αₑ = 0 | case 2, diffuse reflection, adiabatic wall |
| αₜ = 1, αₑ = 1 | case 3, diffuse reflection, constant T_w |

**Hydrogen-air propellant**

*Axisymmetric conical nozzle*

| A=100, α = 15° |
| P₀ = 0.1 atm |
| P₀ = 0.5 atm |
| P₀ = 1.0 atm |

**Thermal Relaxation**

| Zᵥ(T₀), Zᵣ(T₀) | temperature-dependent |
| Zᵥ=100, Zᵣ=5 | moderate relaxation |
| Zᵥ = Zᵣ = 1 | fast relaxation |
Table 3.5. Calculated performance characteristics for nitrogen flow in axisymmetric conical nozzle, $A = 100$, $\alpha = 20^0$, $T_0 = 1,033$ K, $T_w = 500$ K, $\alpha_E = 1$, $\alpha_d = 1$

<table>
<thead>
<tr>
<th>Re</th>
<th>$F$, mN</th>
<th>$I_{sp}$, sec</th>
<th>$\eta$, %</th>
</tr>
</thead>
<tbody>
<tr>
<td>178</td>
<td>5.48</td>
<td>116.2</td>
<td>80.7</td>
</tr>
<tr>
<td>306</td>
<td>8.70</td>
<td>119.9</td>
<td>83.3</td>
</tr>
<tr>
<td>409</td>
<td>11.76</td>
<td>122.4</td>
<td>85.0</td>
</tr>
</tbody>
</table>

Table 3.6. Flow conditions

<table>
<thead>
<tr>
<th>Set</th>
<th>$T_0$, K</th>
<th>$T_t$, K</th>
<th>$p_t$, Pa</th>
<th>$u_t$, m/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>300</td>
<td>250</td>
<td>5,270</td>
<td>322.4</td>
</tr>
<tr>
<td>2</td>
<td>1,000</td>
<td>833</td>
<td>23,820</td>
<td>586.2</td>
</tr>
<tr>
<td>3</td>
<td>2,000</td>
<td>1,667</td>
<td>56,351</td>
<td>819.2</td>
</tr>
</tbody>
</table>

Table 3.7. Calculated performance characteristics for axisymmetric conical nozzle, $A=100$, $\alpha = 15^0$, $N_2$

<table>
<thead>
<tr>
<th>Case</th>
<th>$T_0 = 300$ K</th>
<th>$T_0 = 1,000$ K</th>
<th>$T_0 = 2,000$ K</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$I_{sp}$, sec</td>
<td>$I_{sp}$, sec</td>
<td>$I_{sp}$, sec</td>
</tr>
<tr>
<td>Ideal</td>
<td>76.5</td>
<td>142.1</td>
<td>201.0</td>
</tr>
<tr>
<td>1</td>
<td>74.8</td>
<td>138.2</td>
<td>194.5</td>
</tr>
<tr>
<td>2</td>
<td>64.2</td>
<td>117.6</td>
<td>166.8</td>
</tr>
<tr>
<td>3</td>
<td>65.5</td>
<td>103.8</td>
<td>141.3</td>
</tr>
<tr>
<td>$\eta$, %</td>
<td>100</td>
<td>97.3</td>
<td>96.7</td>
</tr>
<tr>
<td>$\eta$, %</td>
<td>79.8</td>
<td>82.7</td>
<td>83.0</td>
</tr>
<tr>
<td>$\eta$, %</td>
<td>83.1</td>
<td>73.0</td>
<td>70.3</td>
</tr>
</tbody>
</table>
Table 3.8. Adiabatic flame temperature and mole fractions for different chamber pressures

<table>
<thead>
<tr>
<th>$p_0$, atm</th>
<th>$T_{ad}$, K</th>
<th>$\chi_{N_2}$</th>
<th>$\chi_{H_2O}$</th>
<th>$\chi_{H_2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>2302</td>
<td>0.667</td>
<td>0.311</td>
<td>0.022</td>
</tr>
<tr>
<td>0.5</td>
<td>2366</td>
<td>0.663</td>
<td>0.320</td>
<td>0.017</td>
</tr>
<tr>
<td>1.0</td>
<td>2390</td>
<td>0.661</td>
<td>0.324</td>
<td>0.015</td>
</tr>
</tbody>
</table>

Fig. 3.3. Axial velocity profile at the throat of the axisymmetric nozzle.
Fig. 3.4. Density fields \((kg/m^3)\) for uniform and nonuniform throat conditions.
Fig. 3.5. Axial velocity profile along the axis of the axisymmetric nozzle.
Fig. 3.6. Translational temperature profiles ($K$) in 3D micronozzle. SMILE solution for different number of particles.
Fig. 3.7. Velocity component $U_x$ profiles ($m/sec$) in 3D micronozzle. SMILE solution for different number of particles.
Fig. 3.8. Density contours in axisymmetric micronozzle. SMILE - upper part, GASP - bottom.
Fig. 3.9. Comparison of the density profiles along the nozzle axis, axisymmetric case.
Fig. 3.10. Velocity component in X direction \((m/sec)\) in axisymmetric micronozzle obtained by SMILE (top) and GASP (bottom).
Fig. 3.11. The X-component of velocity at the nozzle exit plane in axisymmetric case.
Fig. 3.12. The $X$-component of velocity along the nozzle axis in axisymmetric case.
Fig. 3.13. Translational temperature contours in K for axisymmetric micronozzle computed with SMILE (top) and GASP (bottom).
Fig. 3.14. Comparison of temperature profiles along the nozzle axis for axisymmetric case.
Fig. 3.15. Density contours ($kg/m^3$) in a flat micronozzle computed for a 3D (top) and 2D (bottom) cases by the DSMC method.
Fig. 3.16. Pressure contours (Pa) in a flat micronozzle computed for the 3D (top) and 2D (bottom) cases by the DSMC method.
Fig. 3.17. Contours of velocity component in X direction (m/s) for a flat micronozzle calculated using the 3D (top) and 2D (bottom) models.
Fig. 3.18. Translational temperature contours (K) for a flat micronozzle calculated using the 3D (top) and 2D (bottom) models.
Fig. 3.19. Mean free path contours (m) for a flat micronozzle calculated using the 3D (top) and 2D (bottom) models.
Fig. 3.20. Viscous layer growth in a flat micronozzle obtained by 3D SMILE.
Fig. 3.21. Translational temperature profile along the nozzle axis for the axisymmetric and 3D nozzles.
Fig. 3.22. X-component velocity profile along the nozzle axis for the axisymmetric and 3D nozzles.
Fig. 3.23. Translational temperature profiles along the nozzle axis for different $\alpha_r$ in an axisymmetric micronozzle.
Fig. 3.24. Translational temperature contours in the symmetry plane of a 3D micronozzle for $\alpha_r = 0.8$ (top) and $\alpha_r = 1$ (bottom).
Fig. 3.25. Density contours in the symmetry plane of a 3D micronozzle for $\alpha_{\tau} = 0.8$ (top) and $\alpha_{\tau} = 1$ (bottom).
Fig. 3.26. Total impulse flux at different axial locations inside a 3D micronozzle.
Fig. 3.27. Translational temperature contours for $Re = 178$.

Fig. 3.28. Calculated and measured nozzle efficiency
Fig. 3.29. Translational temperature fields for Set 1.

Fig. 3.30. Translational temperature along the nozzle centerline for Set 1.
Fig. 3.31. Translational temperature fields for Set 2. Case 1 - specular reflection, Case 2 - diffuse reflection, adiabatic wall, Case 3 - diffuse reflection, $T_w=300$ K.

Fig. 3.32. Translational temperature along the nozzle centerline for Set 2.
Fig. 3.33. Translational temperature fields for Set 3.

Fig. 3.34. Translational temperature along the nozzle centerline for Set 3.
Fig. 3.35. Normalized thrust at different axial stations for three throat conditions.
Fig. 3.36. Normalized density for $T_0 = 1000$ K (top) and 300 K (bottom).
Fig. 3.37. Velocity in X direction along the nozzle centerline; full accommodation at the wall.
Fig. 3.38. Translational temperature normalized by its value at the throat for hydrogen-air propellant, conical nozzle, $A = 100$, $\alpha = 15^0$, $p_0 = 0.1$ atm (top) and $p_0 = 0.5$ atm (bottom).
Fig. 3.39. Specific impulse at different axial stations for different chamber pressures.
Fig. 3.40. Specific impulse at different axial stations for $p_0 = 1$ atm and different vibrational relaxation numbers.
Chapter 4

Coupled Fluid-Thermal Analysis of Microthrusters

4.1 Background and motivation

In a high-temperature microthruster, the heat transfer between the gas and the solid wall surfaces may necessitate the cooling of its structure. The concept of a micro-machined bipropellant rocket engine with regeneratively cooled walls was introduced in Ref. [61, 62]. In that work, it was emphasized that the heat flux and heat load limits are two major physical design constraints for micropropulsion devices.

The nozzle wall temperature and heat fluxes are major factors that influence the gaseous flow dynamics and thruster performance, yet the temporal variation of the thruster temperature is often an unknown in the system design. The burn time of the thruster is an important design parameter which determines the impulse bit which will be available for a spacecraft propulsion maneuver. However, the heating of the microthruster structure due to the heat transfer between the high-temperature supersonic flow in the nozzle and thruster walls imposes time limits on its operation, and consequently on the total impulse.

To accommodate the above constraints, a general capability to model coupled, time-dependent fluid and thermal behavior in micro-combustion devices is required. The results of the comparison of DSMC calculations from Section 3.3.1 of heated hydrogen flow in an axisymmetric nozzle with the experimental data, showed that the flow is
strongly non-adiabatic. The DSMC results are in good agreement with the experimental data if a wall temperature of $T_w = 500$ K is assumed. The numerical results for the specific impulse efficiency were found to agree with the experimental data for Reynolds numbers of 178, 306 and 409 within 0.5% agreement. However for a lower wall temperature of 300 K and an adiabatic wall model, the simulation significantly overestimates the data.

In this chapter, a coupled fluid and thermal model is applied for to the modeling of fluid flow in a MEMS device. The developed computational tool allows the accurate computation of wall heat fluxes, temporal variation of the gas flow, and other system parameters without having to specify the unknown wall temperature. The nozzle material thermal response can be expected to have an impact on micronozzle integral quantities such as thrust, specific impulse efficiency and system specifications such as the maximum operational burn time. The model and computational approach is applied to a prototype micropropulsion system designed at NASA Glenn Research Center. The outline of the chapter is following. Section 4.2 describes the proposed approach to coupled thermal and fluid analysis of high-temperature gas microthruster. Section 4.3 presents and discusses the numerical study of the effects of flow three-dimensionality, Reynolds number and wall cooling conditions on the performance of the prototype thruster. The finding presented in this chapter were published in parts in Refs. [4, 5].

4.2 Modeling approach

The proposed modeling approach is based on the solution of the transient conduction heat transfer problem coupled with the DSMC solution of the gas flow inside a
thruster. At the interface between the solid microthruster material and the gas inside
the nozzle, a heat transfer can occur if the stagnation temperature of the gas is different
than the temperature of the solid. Typically, the initial temperature of the material is
at 300 K and if a high-temperature gas is generated in the thruster by, for example, a
combustion process, the heat transfer from the gas to the solid material will occur. As
a result the solid material temperature will increase. The temperature of the gas-solid
surface interface (wall temperature) is in turn an important factor affecting gas flow in
the microthruster. Therefore, the problem of the conduction heat transfer in the thruster
material and gas flow inside the thruster are coupled and has to be solved simultaneously.

In this approach, the coupling between the material thermal response and fluid
flow is carried out by using the DSMC calculated heat fluxes as the boundary condition in
the heat conduction problem at the gas-solid interface. The wall temperature calculated
in the heat transfer simulation is in turn applied in the gas flow simulation.

Let us first estimate the characteristic time scales involved in the transient heat
transfer problem in a microthruster. The first time scale is associated with the gas flow
in the micronozzle, $\tau_g$. This time scale is equal to the residence time of a gas molecule in
the nozzle or $\tau_g = L_s / u_s$ where $L_s$ is the characteristic length scale and $u_s$ is the velocity
scale. The second time scale in the coupled heat transfer problem is the time constant
for the heat transfer in the solid material, $\tau_s$. The time scale $\tau_s$ can be estimated by
using the lumped capacitance method [38] since the Biot number for microscale devices
is small. Using the lumped capacitance method $\tau_s = \rho_s L_s c_{p,s} / h_g$ where $\rho_s$, $c_{p,s}$ - solid
density and specific heat at constant pressure, and $h_g$ is the gas convective heat transfer
coefficient. For example, if $L_s=100 \mu m$, $h_g = 10 W/m^2 \cdot K$, and density, specific heat
for silicon, then $\tau_s \approx 10^{-2}$ sec. If the gas is, say, nitrogen at 2000 K, then $\tau_g \approx 10^{-7}$ sec. Thus, for a typical microthruster the time scale of the gas flow is much smaller than that for the heat conduction in the solid material.

Therefore, a steady state solution for the gas flow is obtained with the DSMC method, and the DSMC results are then used to update the wall temperature boundary conditions in the finite-element heat transfer calculations. The unsteady calculations of conduction heat transfer are then carried out until the wall temperature changes by a significant amount. The calculated wall temperature are then used for a new DSMC calculation of the gas flow and a new cycle of the coupled calculations is repeated.

To analyze the impact of the update frequency, the computations of a one-dimensional heat conduction problem were performed. Figure 4.1 shows the temporal variation of the wall temperature at the gas-surface interface for this problem. Three different criteria for temperature increments are used here, namely, 5%, 10% and 20% of the initial wall temperature. Since the difference in the wall temperature among the three test cases was only a few degrees, a 10% increment was used for the two-dimensional and three-dimensional coupled calculations presented in this chapter.

### 4.2.1 Finite element method for heat conduction equation

The thermal response of the solid structure is governed by the heat transfer equation:

$$\frac{\partial (\rho c_p T)}{\partial t} = \nabla \cdot (k \nabla T) \quad \text{on } \Omega \quad (4.1)$$
where \( T \) is the temperature, \( \rho \) is the density, \( c_p \) is the specific heat at constant pressure, \( k \) is the thermal conductivity, and \( \Omega \) is the domain. The boundary conditions for the problem are

\[
T \bigg|_{\Gamma_1} = T_1, \quad k \frac{\partial T}{\partial n} \bigg|_{\Gamma_2} = q_a + q_c + q_r
\]

where \( q_a \) is the conduction heat flux, \( q_c = h(T - T_2) \) is the convective heat flux, \( q_r \) is the radiative heat flux, \( T_1 \) is the given temperature on the boundary, and \( T_2 \) is the known ambient temperature, \( \Gamma_1 \cup \Gamma_2 = \partial \Omega \) is the boundary of the domain, and \( n \) is the normal unit vector to the boundary.

The numerical solution to the heat conduction problem can be obtained by the finite element method [73] which is especially suitable for problems involving complex geometries. In this work, triangular and tetrahedral elements with linear interpolation functions have been used in the finite element solution for the two-dimensional and three-dimensional models of the micro-nozzle, respectively. The unstructured grids were constructed using the GRIDGEN code [32]. Figure 4.2 shows the triangular grid for 2D microthruster configuration. The mesh has 643 nodes and 1174 triangular elements. The 3D mesh has 1627 nodes and 7291 tetrahedral elements.

The time integration in the transient heat conduction calculations is carried out using a first-order purely implicit scheme. The solution of the system of linear algebraic equations resulting from the finite element formulation is obtained by a Lower/Upper triangular (LU) decomposition. An object oriented Java code has been developed for the finite element method implementation of the 2D and 3D heat transfer problem.
The details of the finite-element formulation for heat conduction problem are as follows. The spatial discretization of the computational domain for the heat transfer calculations is based on the Galerkin finite element algorithm [73]. When the heat transfer equation is multiplied by weighting functions $N$, and then integrated over the domain $\Omega$, one gets the following equation:

$$\int_{\Omega} N \cdot \nabla (k \nabla T) d\Omega = \int_{\Omega} N \cdot \rho c_p \frac{\partial T}{\partial t} d\Omega \quad (4.2)$$

where $\Omega$ is the computational domain, and $N$ are weighting functions. Then applying the divergence theorem, the above equation takes the form:

$$\int_{\Omega} \nabla N \cdot k \nabla T d\Omega + \int_{\Omega} \rho c_p N \frac{\partial T}{\partial t} d\Omega = \int_{\Gamma} N k \nabla T \cdot \vec{n} d\Gamma \quad (4.3)$$

where $\Gamma$ is the boundary of this domain.

The computational domain is divided into the triangle elements in 2D case, and the tetrahedral elements in 3D case. Temperature $T$ is approximated by a linear combination of weighting functions $N$ and values of the temperature in the nodes of the elements:

$$T(x, y, z, t) = \sum_{e} N^e(x, y, z) T_e(t) \quad (4.4)$$

When linear approximation functions $N$ are applied to triangular and tetrahedral elements, the integral equation (4.3) can be discretized as:

$$\sum_{e} \int_{\Omega_e} k (N_x \cdot N^e_x + N_y \cdot N^e_y + N_z \cdot N^e_z) d\Omega_e \cdot T_e$$
or in matrix notations:

\[ M\dot{T} + KT = q \]

where \( \dot{T} \) is the time differentiation.

The system can be integrated in time using the purely implicit scheme as

\[ (M + \Delta tK)\Delta T^{(n+1)} = \Delta t(q - KT^{(n)}) \]

where \( T^{(0)} \) is the initial domain temperature and \( T^{(n)} \) is the domain temperature at the \( n \)-th time step.

4.3 Simulations

4.3.1 Microthruster geometry and flow conditions

To study the coupled heat transfer and gas flow problem in a high-temperature micropropulsion applications, the numerical simulations are carried out for a microthruster designed by NASA Glenn researchers. A schematic of the single microthruster modeled here and axis notations used henceforth are shown in Fig. 4.3. The dimensions of the outer surfaces of the thruster are as shown in the figure. The micronozzle has a throat width of 300 \( \mu m \), a depth of 600 \( \mu m \) and a length of 250 \( \mu m \). The converging part of the nozzle has a half-angle of 30 deg and the inlet to throat area ratio of 10. The expansion half-angle of the diverging part is equal to 15 deg with an exit to throat area ratio of 5. Two-dimensional and three-dimensional models of this nozzle were considered. The 2D
nozzle corresponds to a cut of the 3D geometry parallel to the x-y plane with infinite height, h. In the discussion of the 3D results, the term “side-wall” will be used. This refers to the x-y planes at z=0 and z=h of the 3D nozzle.

The high-temperature flow inside the proposed microthruster will be generated by a laser-ignited solid mono-propellant decomposition. In the present modeling study, the flow of molecular nitrogen, one of the major components of the decomposition products, was simulated at the stagnation pressures of 0.1 and 0.5 atm and a stagnation temperature of 2,000 K. The Reynolds number based on the throat width of 300 $\mu\text{m}$ is equal to 35 and 175 for these two pressures, respectively.

4.3.2 Thermal conditions

Two conditions at the external boundary of the microthruster have been studied, zero heat flux (thermally insulated conditions, $q_a = q_c = 0$) designated as no heat removal and convective heat flux $q_c = h(T - T_\infty)$ designated as cooling. The latter corresponds to the situation where the microthruster wall is actively cooled by a liquid flow with a heat conduction coefficient $h = 10^3 \text{ W/m}^2 \cdot \text{K}$ and freestream temperature of 300 K. Such a heat conduction coefficient is typical for laminar water flow cooling in microchannels [47]. The liquid flow active cooling was modeled assuming that it is used along the perimeter of the rectangular material shape. The thermal properties of the silicon nozzle material were assumed to be constant at $k = 1.412 \text{ W/cm} \cdot \text{K}$, $c_p = 0.7 \text{ J/kg} \cdot \text{K}$, and $\rho = 2.33 \text{ g/cm}^3$. The microthruster material temperatures are limited by the melting temperature of silicon which is sufficiently low so that radiative heat fluxes can be neglected ($q_r = 0$). A heat transfer calculations with radiative cooling of the outer
thruster surface to an atmospheric temperature of 300 K and an emissivity of 0.5 were also performed. Comparison of the heat transfer calculations for $p_0 = 0.5 \text{ atm}$ without convective cooling and with and without radiation heat flux showed only negligible (<10 K) differences in the predicted material temperature.

4.3.3 2D simulation results

As a demonstration of the coupled heat transfer and transitional flow calculations we first considered a two-dimensional heat transfer calculation. The nozzle depth is assumed infinite in this case. The 2D results may provide important information on the effect of fluid/thermal coupling. However, as the gas flow develops towards the exit, the viscous boundary layer grows in all three dimension. Hence, a fully three-dimensional, coupled, time-dependent heat transfer calculation should be obtained before final system conclusions may be drawn.

The coupled calculations have been performed using the T-Rex Linux cluster at Penn State consisting of 48 dual Athlon 1.0 GHz processor nodes. A typical CPU time for a single DSMC calculation of a 2D microthruster flow at $p_0 = 0.1 \text{ atm}$ is two hours using 10 processors. A typical CPU time for a single transient 2D heat conduction calculation is a few minutes using a single processor.

Material thermal response

Figures 4.6 and 4.7 show the temporal evolution of the temperature in the gas flow and in the solid material for the two thermal boundary conditions under consideration and a stagnation pressure of 0.1 atm. These and succeeding figures show the gas
translational temperature since the rotational temperature closely follows the translational one, and the vibrational energy is a small fraction of the total gas flow energy.
The initial material temperature was assumed to be 300 K hereafter. It is seen that the flowfield structure and the material temperature changes significantly with time. For the thermally insulated case, the material temperature increases from 300 K to 1200 K over about 14 s. The calculation was stopped after the material temperature reached 1200 K, the value close to the melting temperature of silicon. It is interesting that the temperature inside the solid material is approximately the same at any fixed time moment (the maximum change is about 10 K). This is primarily due to the very small dimensions of the thruster. The heat flux to the surface decreases with time as the difference between the gas and the surface temperatures becomes smaller. This, in turn, somewhat slows the temporal rate of change of the material temperature.

**Gas flowfield structure**

The change in the gas flow structure is determined by the change in the wall surface temperature. Initially, the flowfield is typical for a cold wall micronozzle. The temperature of the gas near the wall is lower than that at the nozzle centerline (X-axis). As the material temperature increases with time, the structure of the converging part of the flow does not change qualitatively. In the diverging part, the temperature maximum shifts from the centerline toward the surface.

In the case of applied cooling, Fig. 4.7, the outer boundary of the material is cooled, and the cooling does not allow the material temperature to reach the melting point for the flow conditions under consideration. In this case, therefore, the coupled calculations were carried out in time until the steady state is reached. Note that the
initial temperature field at time zero is not shown here since it coincides with that in Fig. 4.6. The steady-state temperature in the material in this case is about 450 K. Even this relatively small change in the nozzle material temperature causes a change in the boundary layer structure.

Let us now consider a higher stagnation pressure case. The temporal evolution of the gas and material temperature for $p_0 = 0.5$ atm is shown in Figs. 4.8 and 4.9 for the two different thermal boundary conditions at the outer thruster surface. The principal difference from the lower pressure flow is due to the higher heat flux from the gas to the surface. The heat flux is higher by a factor of about 2.6, as explained below in greater detail. This causes a larger change of temperature inside the solid material (about 30 K), that is still small compared to the variations in the gas flow. The relatively high heat flux also results in a change in the time necessary to reach the melting temperature for insulated case. It is about 6 s for $p_0 = 0.5$ atm (cf. to 14 s for $p_0 = 0.1$ atm). For cooling, even with the higher stagnation pressure the material does not reach the melting temperature due to the applied cooling. The steady-state material temperature for this case is about 700 K. The change in the gas flow structure as a function of time is qualitatively similar to the lower pressure case. However in the higher pressure case, the boundary layer thickness is much smaller both in diverging and converging parts. Also, there is a temperature minimum in the diverging part between the surface and the centerline.

The variation of the heat flux from the gas to the solid surface versus the distance along the wall is plotted in Figs. 4.10 and 4.11 for the two stagnation pressures of 0.1 and 0.5 atm, respectively for Case 1. The maximum heat flux value for both pressures
is at the nozzle throat (location of the throat is shown in Fig. 4.10 by dotted lines). The heat flux for \( p_0 = 0.5 \text{ atm} \) is about 2.6 times higher than that for \( p_0 = 0.1 \text{ atm} \). The heat flux is not proportional to the stagnation pressure due to a higher heat transfer coefficient in the gas for the more rarefied case, \( p_0 = 0.1 \text{ atm} \).

The gas flowfield inside the microthruster is more sensitive to the change in wall temperature for the lower pressures, due to larger surface effects for the lower Reynolds number case. Figures 4.12 and 4.13 shows the translational temperature profiles at the nozzle exit for insulated case and two different stagnation pressures, 0.1 and 0.5 atm, respectively. For \( p_0 = 0.5 \text{ atm} \), the temperature at the center line (\( Y=0 \)) changes by less than 80 \( K \) with the wall temperature changing from 300 K to 1200 K, whereas for the lower pressure \( p_0 = 0.1 \text{ atm} \) the change is more than 400 \( K \). The X-component of velocity profiles at the exit are plotted in Figs. 4.14 and 4.15 for stagnation pressure of 0.1 and 0.5 atm, respectively. For the lower pressure case, the velocity increases with time due to the greater influence of the wall temperature. For the higher pressure, the velocity almost does not change. The change in the wall temperature has the greatest effect on the gas density field. The density profiles at the exit are shown in Figs. 4.16 and 4.17 for the two pressures. The density changes by as much as 100 \% for both pressures as the wall temperature increases from 300 K to 1200 K.

The temporal variation of Mach number contours for insulated case and stagnation pressure \( p_0 = 0.1 \text{ atm} \) is shown in Fig. 4.18. As the time progresses, the Mach number decreases due to higher temperatures and a thicker wall boundary layer. The Mach number is 2.7 at \( t=0 \) and 2.3 at \( t=9.5 \text{ s} \).

**Micronozzle performance**
Consider now how the performance characteristics of the micronozzle such as mass discharge coefficient, thrust and specific impulse, change in time as the wall temperature increases. The temporal variation of the thrust for the two-dimensional cases under consideration is given in Fig. 4.19. The thrust values here are normalized by the initial value at $t = 0$ for a constant wall temperature of 300 K. For the lower stagnation pressure case, the initial value of the thrust is 2.0 mN, and for $p_0 = 0.5$ atm the value is 12.5 mN (assuming the nozzle height in the Z direction is 600 $\mu m$). The thrust decreases in time in all four cases due to the higher temperatures and thus larger viscous losses, though the decrease in thrust is small. For the zero heat flux at the external boundary case, the final value of thrust is about 2% lower than its initial value, and for the case of applied cooling the final value is 3% lower.

The amount of the flow energy that is lost to the wall in the form of heat can be estimated from the total energy fluxes in the nozzle. The total energy flux is given in Fig. 4.20 for the cooling case and a stagnation pressure of 0.5 atm as a function of the distance from the nozzle inlet. The total energy flux is calculated as the sum of the flow kinetic and internal energy fluxes through a section perpendicular to the nozzle axis. It is normalized by its value at the inlet. For $t=0.3$ sec the inlet value is 35.2 kW, and at $t=10.3$ sec, it is 33.3 kW. The flux of the total flow energy has to be conserved in an adiabatic case when there is no heat transfer between the gas and the solid wall. Figure 4.20 shows that for the case of applied cooling, a non-adiabatic condition, the energy flux is decreasing along the $X$-axis. Thus, the heat transfer losses in the micronozzle are about 35 % for $t=0$ sec and about 29 % at $t=10.3$ sec.
The reason that the thrust of the micronozzle decreases even though the heat transfer losses are decreasing is that the mass discharge coefficient becomes smaller with time. The ratio of the mass flow to the ideal mass flow for the four two-dimensional cases is plotted in Fig. 4.21, each normalized by its initial value at $t=0$. The initial values of mass discharge coefficient are 0.89 and 0.94 for stagnation pressures of 0.1 and 0.5 atm, respectively. The mass discharge coefficient decreases in time because for higher gas temperatures, the thickness of the wall boundary layer increases, thus diminishing effective nozzle throat area. The largest decrease in mass discharge occurs at the lower pressure in insulated case where the final value of the discharge coefficient is 21 % less than the initial one.

4.4 3D simulation results

In this section results of the numerical simulation using DSMC and finite element methods of a gas flow and heat transfer in a 3-D microthruster under different flow conditions are presented. The cases that are considered here are summarized in Table 4.1. The simulation in each case involved transient heat transfer calculations coupled to DSMC solutions for the gas flow inside the nozzle. The coupled calculations have been performed using a Linux cluster at Penn State consisting of 48 dual Athlon 1.0 GHz processor nodes. A typical CPU time for a single DSMC calculation of a 3D microthruster flow at $p_0 = 0.1$ atm is four hours using 56 processors. A typical CPU time for a single transient 3D heat conduction calculation is a few minutes using a single processor.

The transient calculations are needed to establish the variation of the wall temperature with time and the operational time limit of the microthruster. The maximum
operational time is the time it takes for the material temperature to reach a value close to the melting temperature where the structural integrity of the devices may be compromised. For each considered case the flow structure inside the micronozzle was analyzed and performance characteristics such as mass discharge and thrust were calculated as a function of time.

4.4.1 Numerical accuracy

The DSMC numerical solution depends on three main parameters: the cell size $\Delta x$, time step $\Delta t$, and the number of particles $N_\lambda$ in a volume with linear size equal to the local mean free path [39]. In the DSMC algorithm, the cell size has to be less than the local mean free path and the time step should be less than the average time between collisions and a residence time in a cell. An even more strict requirement is that the number of simulated particles has to be large enough to ensure that the statistical correlations between particles are insignificant. All three requirements were satisfied in the calculations for $p_0 = 0.1$ atm where the linear size of a background cell was taken as $20 \, \mu m$ with four partition levels of grid adaptation, a time step of $1.8 \times 10^{-9}$ s, and total of about 2.8 million simulated particles.

For the higher stagnation pressure of 0.5 atm, the DSMC method requirements for cell size, time step and number of particles are hard to satisfy rigorously. Therefore, the calculations have been conducted with different time steps and numbers of particles. The calculations with different time steps showed that the results do not change for $\Delta t = 1, 2, 4 \times 10^{-9}$ s. The results of calculations with the different total numbers of particles of about 15 and 30 million and 3 and 5 million collision cells are shown in
Figs. 4.4 and 4.5. The temperature and X-component of velocity inside the micronozzle are in satisfactory agreement and the maximum difference among the three solutions is less than 3%. The ratio of real to simulated particles for the all 3-D calculations with \( p_0 = 0.5 \) atm presented below was the same as in the case with 13 million particles.

### 4.4.2 Effects of the Reynolds number

Let us now consider the effects of the Reynolds number on the flow structure and thermal behavior of the micronozzle. Two nominal Reynolds number cases defined by conditions at the throat are considered, 35 and 175, which correspond to stagnation pressures of 0.1 (Case 1) and 0.5 atm (Case 4), respectively.

For the lower pressure case, the gas expansion inside the nozzle is hindered by a thicker boundary layer. Figure 4.27 shows the Mach number profile along X-axis for Cases 1 and 4 at t=0 \( (T_w = 300 \) K). The Mach number in the diverging portion of the micronozzle is significantly less for Case 1 than for Case 4 and the value of the Mach number at the exit is about 1.9 and 2.4 for the two stagnation pressures 0.1 and 0.5 atm, respectively.

The temperature fields for Case 1 and Case 4 are plotted in Figs. 4.23 and 4.28, respectively. The principal difference between the flows for the two Reynolds number cases is due to the change in the heat flux from the gas to the surface. The heat flux in Case 4 is higher by a factor of about 2.6 than in Case 1. This causes a larger change of temperature inside the solid material (about 30 K), that is still small compared to the temperature variation in the gas flow. The higher heat flux in Case 4 results in a shorter
time that it takes the material to reach the melting temperature for Case 1. It is about 6 s for Case 4 (cf. to 14 s for Case 1).

4.4.3 Effects of thermal boundary conditions

The effects of cooling applied on the microthruster outer surface can be illustrated by comparison of the calculations for Case 1 and 2, and Case 4 and 5. Figures 4.23 and 4.24 show the temperature fields in the Z=0 plane for Cases 1 and 2, respectively. As one can see the temperature inside the microthruster material increases with time for both cases but by cooling the outer surface of the thruster in Case 2, it is possible to sustain the thruster material temperature at a level which is lower than the melting temperature. Similar influence of the applied cooling is observed in Case 4 and 5 (see Figs. 4.28, 4.29). The material temperature reaches a value of 1,200 K in about 13 sec for Case 1 (see Fig. 4.23) and in about 3 sec for Case 4 (Fig. 4.28). But in the cases with applied cooling the calculated steady state material temperature is about 450 K and 650 K in Cases 2 and 5, respectively.

Hence, the cooling allows for a longer thruster burn-time. For both stagnation pressures the cooling results in higher mass flow rate and thrust as a function of time (see Table 4.2).

4.4.4 Effects of the geometric shape

The influence of the geometric shape of the microthruster, in particular, its height, on the flow structure and thermal material response can be studied by comparison of Case 1 and 3 and a corresponding 2-D case.
The comparison between the X-component of velocity profiles in Case 1 ($h = 600 \, \mu m$), Case 3 ($h = 1,200 \, \mu m$) and a 2D case that corresponds to infinite height $h$ is shown in Figure 4.22. All three cases are for a wall temperature of 300 K ($t=0$). Figure 4.22 shows that the height of the microthruster has a significant effect on the gas expansion inside the micronozzle. In particular, the X-velocity at the exit for the lowest height is about 55% of the velocity in the corresponding 2D case. The nozzle efficiency increases by doubling the height because the velocity at the exit is 82% of the velocity in the 2D case.

The difference in the thermal response of the material for a microthruster with different heights is illustrated in Figs. 4.23 and 4.26 where the temperature field in the $Z=0$ plane is plotted for Cases 1 and 3, respectively. As one can see, the thruster material temperature reaches 1,200 K in about 8 sec in Case 3 compared to 13 sec in Case 1. This is due to the larger area of the interface between the material and high-temperature gas flow and a smaller overall volume of material in Case 3.

4.4.5 Microthruster performance

Let us now consider the temporal variation of the microthruster performance for the three-dimensional case. Calculated performance parameters of the 3D microthruster are listed in Table 4.2. For all considered cases both thrust and mass discharge coefficient decrease in time with increasing material temperature.

The mass discharge coefficient decreases in time because of the increase of the thermal boundary layer as the wall temperature increases. The density in the thermal boundary layer is decreased as well as flow velocity and thus the mass flow is diminished.
A similar influence of the thermal wall boundary conditions on mass discharge was obtained in Ref. [46] for higher Reynolds numbers from 2,000 to 20,000.

The thrust of the micronozzle decreases with time much more significantly than in the two-dimensional case due to higher viscous and heat transfer losses. For the lower stagnation pressure, $p_0 = 0.1$ atm, the final thrust value are 15% and 6% smaller than the initial values for Case 1 and 2, respectively. The corresponding decrease of the thrust in the two-dimensional case is only 2-3%.

The large temporal variation of the thrust and especially, mass discharge coefficient in such microthrusters predicted by these simulations means that the coupling between gas flow and material thermal response has to be taken into account in micropropulsion system design.

### 4.5 Summary

A coupled thermal and fluid analysis of a 2D and 3D micronozzle was presented. The nozzle silicon material thermal response was modeled as a solution of the transient heat conduction equation which is obtained by the finite element method. The gas flow solution was obtained by the direct simulation Monte Carlo method for $Re = 35$ and 175 corresponding to chamber pressures of 0.1 and 0.5 atm. Since the time scale for gas flow is much shorter than the thermal response time, the steady state solutions of the flow parameters were used. DSMC calculated heat fluxes at the gas-solid interface were applied as a boundary condition to the heat conduction in the solid. The DSMC calculations of the flow and the heat flux to the surface were repeated when the wall temperature changed by 10%. In this manner it was possible to obtain the temporal variation of
the material temperature and gas flowfields without having to specify the unknown final wall temperature. The true thermal environment of the microthruster will depend on the final systems configuration and platform integration. However, to understand the systems effects due to thermal-fluid coupling, two different thermal boundary conditions were considered. The first case considered corresponds to that of a thermally insulated condition whereby the convective and conductive heat fluxes were assumed to be zero. The second thermal condition corresponded to that of a nozzle actively cooled by a liquid flow about the perimeter of the nozzle such that the nozzle material conducted heat to a free stream temperature of 300 K.

The material temperature response and the gas flowfields were studied for the 2D model for the two stagnation pressures and two thermal conditions. Both the flowfield temperature field structure as well as the material temperature changed significantly as a function of time. For the adiabatic case at the lower stagnation pressure, the material temperature changed from its initial value of 300 K to 1200 K (the value close to the melting point of silicon) over about 14 s. The structure of the converging part of the flow did not qualitatively change, however, there are significant changes in the flow structure in the diverging portion of the nozzle as the viscous boundary layer grows. Although the material steady state temperature only reaches ~ 450 K for the second thermal condition, the flow boundary layer structure changed as a function of time. For the higher pressure case, the change in the gas flow structure as a function of time is qualitatively similar to that of the lower pressure case. It was seen, however, that in the higher pressure case, the boundary layer thickness was smaller both in the diverging and converging portions of the nozzle gas flow.
Table 4.1. Summary of cases considered

<table>
<thead>
<tr>
<th>Case</th>
<th>$p_0$, atm</th>
<th>$h$, $\mu m$</th>
<th>Thermal conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.1</td>
<td>600</td>
<td>no heat removal</td>
</tr>
<tr>
<td>2</td>
<td>0.1</td>
<td>600</td>
<td>cooling</td>
</tr>
<tr>
<td>3</td>
<td>0.1</td>
<td>1200</td>
<td>no heat removal</td>
</tr>
<tr>
<td>4</td>
<td>0.5</td>
<td>600</td>
<td>no heat removal</td>
</tr>
<tr>
<td>5</td>
<td>0.5</td>
<td>600</td>
<td>cooling</td>
</tr>
</tbody>
</table>

A single 3D micronozzle model coupled to a full 3D thermal solution was obtained for both thermal conditions. The time dependence of the material thermal response was found to be qualitatively similar to that observed in the corresponding 2D cases. However, the gas flow in both the converging and diverging portions of the nozzle were very different due to the impact of the boundary layer on the side walls in the 3D case.

The predicted thrust and mass discharge coefficient of both 2D and 3D micronozzle models decreases in time as the viscous losses increase for increasing higher wall temperatures. However due to the greater impact of the third surface viscous losses, the decrease in thrust and mass discharge coefficient as a function of time is greater for the
Table 4.2. Calculated performance

<table>
<thead>
<tr>
<th>t, sec</th>
<th>T_{tv}, K</th>
<th>c_d, %</th>
<th>F, mN</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Case 1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>300</td>
<td>0.87</td>
<td>1.44</td>
</tr>
<tr>
<td>2.4</td>
<td>500</td>
<td>0.64</td>
<td>1.33</td>
</tr>
<tr>
<td>7.6</td>
<td>870</td>
<td>0.48</td>
<td>1.27</td>
</tr>
<tr>
<td>12.9</td>
<td>1160</td>
<td>0.41</td>
<td>1.24</td>
</tr>
<tr>
<td>Case 2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.34</td>
<td>340</td>
<td>0.87</td>
<td>1.41</td>
</tr>
<tr>
<td>1.15</td>
<td>390</td>
<td>0.84</td>
<td>1.38</td>
</tr>
<tr>
<td>3.2</td>
<td>440</td>
<td>0.80</td>
<td>1.33</td>
</tr>
<tr>
<td>Case 3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>300</td>
<td>0.88</td>
<td>3.49</td>
</tr>
<tr>
<td>2.0</td>
<td>530</td>
<td>0.75</td>
<td>3.34</td>
</tr>
<tr>
<td>4.18</td>
<td>860</td>
<td>0.66</td>
<td>3.27</td>
</tr>
<tr>
<td>8.2</td>
<td>1170</td>
<td>0.57</td>
<td>3.22</td>
</tr>
<tr>
<td>Case 4</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>300</td>
<td>0.93</td>
<td>9.32</td>
</tr>
<tr>
<td>1.96</td>
<td>800</td>
<td>0.75</td>
<td>9.04</td>
</tr>
<tr>
<td>3.36</td>
<td>1080</td>
<td>0.68</td>
<td>8.99</td>
</tr>
<tr>
<td>Case 5</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.64</td>
<td>480</td>
<td>0.88</td>
<td>9.22</td>
</tr>
<tr>
<td>1.14</td>
<td>530</td>
<td>0.84</td>
<td>9.12</td>
</tr>
<tr>
<td>4.16</td>
<td>650</td>
<td>0.81</td>
<td>9.02</td>
</tr>
</tbody>
</table>
Fig. 4.1. Wall temperature temporal variation for different temperature increments between heat flux updates.
Fig. 4.2. Computational mesh for 2D heat transfer calculations.
Fig. 4.3. Schematic a half-section of the microthruster.
Fig. 4.4. X-component of velocity profile along X-axis for Case 1 (t=0 s, initial thermal conditions) with different total numbers of particles.
Fig. 4.5. Translational temperature profile along X-axis for Case 1 (t=0 s, initial thermal conditions) with different total numbers of particles.
Fig. 4.6. Temperature field for $p_0 = 0.1$ atm, 2D, no cooling
Fig. 4.7. Temperature field for $p_0 = 0.1$ atm, 2D, cooling.
Fig. 4.8. Temperature field for $p_0 = 0.5$ atm, 2D, no cooling
Fig. 4.9. Temperature field for $p_0 = 0.5$ atm, 2D, cooling
Fig. 4.10. Wall heat flux distribution along the surface for $p_0 = 0.1$ atm, 2D, no cooling.

Fig. 4.11. Wall heat flux distribution along the surface for $p_0 = 0.5$ atm, 2D, no cooling.
Fig. 4.12. Translational temperature profiles at the nozzle exit for \( p_0 = 0.1 \text{ atm}, 2D, \) no cooling.

Fig. 4.13. Translational temperature profiles at the nozzle exit for \( p_0 = 0.5 \text{ atm}, 2D, \) no cooling.
Fig. 4.14. X-component of velocity profiles at the nozzle exit for $p_0 = 0.1$ atm, 2D, no cooling.

Fig. 4.15. X-component of velocity profiles at the nozzle exit for $p_0 = 0.5$ atm, 2D, no cooling.
Fig. 4.16. Number density profiles at the nozzle exit for $p_0 = 0.1$ atm, 2D, no cooling.

Fig. 4.17. Number density profiles at the nozzle exit for $p_0 = 0.5$ atm, 2D, no cooling.
Fig. 4.18. Mach number field for $p_0 = 0.1$ atm, 2D, no cooling.
Fig. 4.19. Thrust variation with time for different conditions, 2D.

Fig. 4.20. Total energy flow for $p_0 = 0.1$ atm, 2D, cooling.
Fig. 4.21. Variation of the normalized mass discharge coefficient with time, 2D.

Fig. 4.22. X-component of velocity profile along X-axis for 2D and 3D simulations for Case 1 and Case 3.
Fig. 4.23. Temperature field for $p_0 = 0.1$ atm in $Z=0$ plane for Case 1, 3D calculations.
Fig. 4.24. Temperature field for $p_0 = 0.1$ atm in Z=0 plane for Case 2, 3D calculations.
Fig. 4.25. Comparison of X-component of velocity profile along the nozzle centerline for $p_0 = 0.1$ atm, Case 1 for 2 and 3D models. $T_w = 300$ K represents the wall condition at $t = 0$s.
Fig. 4.26. Temperature field for Case 3 in Z=0 plane.
Fig. 4.27. Mach number profile along X-axis for Cases 1 and 4.
Fig. 4.28. Temperature field for Case 4 in Z=0 plane.
Fig. 4.29. Temperature field for Case 5 in Z=0 plane.
Fig. 4.30. Normalized thrust variation with time for two thermal conditions, 3D calculations, $p_0 = 0.1$ atm.

Fig. 4.31. Variation of the normalized mass discharge coefficient with time, 3D calculations.
Chapter 5

Microchannels with Contraction

5.1 Previous study of gaseous microchannel flows

The pressure-driven gaseous microchannel flow is a basic element of MEMS microfluidic devices. Such flow occurs, for example, in micropumps [84], micro heat exchangers [89] and microengine inlet sections [65]. Rarefied gas flow in channels encountered in vacuum systems has been extensively studied by researchers in rarefied gas community. A comprehensive review covering rarefied flow in circular channels can be found in Ref. [27]. Due to the manufacturing process, microchannels encountered in MEMS have planar geometry. The rarefaction effects in MEMS channels such as non-linear pressure distribution have been extensively studied in the last decade both experimentally [72, 80, 33] and theoretically [9, 14, 71].

The uniform microchannel flow in the slip regime has been treated analytically and experimentally by Arkilic et al [9]. The analytical model was based on a perturbation expansion of the Navier-Stokes equations with first order correction for the wall slip. The authors obtained the following expression for the mass flow for given inlet and outlet pressures of the microchannels:

\[ \dot{m} = \frac{H^3 d p_0^2}{24 \mu LRT} \left( \left[ \frac{p_i}{p_0} \right]^2 - 1 + 12 \alpha_r Kn \left( \frac{p_i}{p_0} - 1 \right) \right) \]  

(5.1)
where $H$, $d$, and $L$ are the channel height, depth, and length; $p_i$ and $p_0$ are the inlet and outlet pressures; $T$, $\mu$ and $R$ are the gas temperature, viscosity and gas constant, respectively. The coefficient $\alpha_T$ represents the streamwise (tangential) momentum accommodation.

The experimental data [8] for nitrogen and helium flows interacting with silicon surfaces suggest that the momentum accommodation coefficient $\alpha_T$ varies from 0.8 to 1.0. The comparison of the experimental measurements of the mass flow with the analytical model predictions that include slip-flow effects (Eq. (5.1)) showed good agreement for Knudsen numbers up to $Kn = 0.165$, whereas, the no-slip solution predicted much lower mass flow levels. A second-order analytical slip-flow model applicable in transitional regime was developed by Beskok and Karniadakis [14]. The limitations of these two analytical models are the assumptions that density and pressure across the channel are constant at any given location and that the temperature effects are negligible (isothermal flow). Due to these limitations the analytical formulas can only be applied to low Mach number flows (typically $M \leq 0.1$).

In the transitional regime, $Kn > 0.1$, obtaining analytical solutions for microchannel flows is very difficult because the approximation of transport terms based on macroscopic quantities becomes unacceptably inaccurate. The DSMC method was applied to study microchannel flow by Piekos and Breuer [71]. The DSMC-computed pressure distributions for an outlet Knudsen number of 0.44 was about 5% smaller than the analytical slip-flow model prediction. The magnitude of both slip and maximum velocity
were greater than the analytical model prediction by as much as 40%. The conclusion made by the authors was that the slip flow analysis begins to fail at approximately Kn=0.15.

Heat transfer characteristics of supersonic uniform microchannels were studied using the DSMC method by Liou and Fang [59] for Knudsen numbers from 0.031 to 0.186. The inlet Mach number was 4.15 in all cases. The flow rarefaction was shown to significantly increase the wall heat transfer coefficient.

The flows through microchannels with constrictions has been discussed by a number of researchers [48, 57, 55, 14]. Karniadakis and Beskok [48] studied the flows over a backwards facing step, through a grooved channel, and into a cavity using DSMC method. The primary emphasis of these calculations was to validate slip-flow correction models. Beskok et al [14] discussed the rarefaction and compressibility effects in microflows emphasizing that both need to be considered if one is to correctly model the physics of microflows. Although the specific configurations of the microchannel devices differ among these researchers [48, 14], the flows share common features in that they were subsonic, of relatively low Reynolds number, and have a Knudsen number in the slip-flow regime (typically between 0.01 and 0.5). It was recognized that due to the finite Knudsen number, the flow field macroparameters, such as, pressure, temperature, and mass flow rate, could not be calculated with the standard continuum, Navier-Stokes formalism.

Zohar and coworkers [57, 55] measured pressure and mass flow rates through microchannel devices with contraction and expansion sections as well as constrictions.
Accurate prediction of mass flow rate and pressure through microchannel systems is critical for establishing a design criteria similar to that of macro devices. In macro systems the total head loss for a system of components with straight and bended or branching portions is well established in terms of tabulated major and minor losses. A concern exists in the design of microdevices that if the flow physics is not entirely understood, it may be difficult to predict whether a specific configuration (composed of straight sections coupled to sections containing constrictions) is optimized from the point of view of minimizing pressure losses. Based on the macrosystem analog, flow separation in microsystem flows containing constriction or bend components could potentially cause large mass flow or pressure losses [55]. Hence, more detailed knowledge about the microflow in terms of accurate velocity fields that illustrate the occurrence of flow separation and the formation and structure of recirculation zones is crucial.

To that end, researchers have tried to elucidate the nature of flow separation and recirculation that can occur in low Reynolds number, subsonic to transonic flows in microdevices. The flow separation is understood to be steady and due, in some nature, to the need for the flow to turn to accommodate a sharp corner (“geometric”) [55, 48, 13]. During this process an adverse pressure gradient can develop, creating a flow condition that may precede separation [78]. However, it was also noted that for such low Reynolds numbers and high channel aspect ratios the flow should exhibit irrotational, Hele-Shaw type [34], features with no flow separation even from sharp corners. Simulation predicted flow separation in shear-driven, grooved microchannels [14], and a backwards step [13] even for low Reynolds numbers, but direct experimental evidence with particle velocity imaging techniques was ambiguous. Hence it has been difficult to sort out the effects of
rarefaction and compressibility factors that may lead to flow separation and the degree of flow recirculation. An important reason for using DSMC method for microchannel flows is that the gas-surface interaction may be exactly specified and controlled to allow one to assess the impact of rarefaction on recirculation. It will be shown in the DSMC calculations of this chapter that for subsonic flows, recirculation will occur due to classical boundary layer arguments.

A series of investigations were undertaken to assess “minor” losses in microflows through non-parallel plate channel configurations [57, 55, 56, 91]. These experimental studies combined MEMS microchannel component fabrication with measurements of not only mass flow rate, but pressure as well. These two simultaneous measurements provide the modeler with important, redundant data that allows one to check for consistency. In particular it was found that in constriction microchannels, the pressure drop just downstream of the constriction decreased to a level much larger than predicted values[55]. The authors, however, were not able to reconcile the large pressure drop with classical flow physics and an explanation for the discrepancy is not provided. It will be shown in this work that the existence of flow separation and the measured pressure drops are consistent. A simple model is presented in the next section to analyze the pressure distributions for a microchannel with constrictions and its accuracy will be assessed by comparison with exact DSMC simulations.

5.2 Analytical model of microchannel with constriction

To obtain the distribution of the flow parameters in a microchannel with constriction in the form of a long microchannel (or a transition section of another shape), one
can consider it as three different flow sections. The first one is a straight microchannel flow upstream of the constriction, the second one is the flow in the transition section, and, finally the straight microchannel flow downstream of the constriction.

For the flow in a microchannel with constriction, the known parameters are inlet and outlet pressures, viscosity coefficient and Knudsen number at the exit as well as geometrical shape of the three sections. A schematic of a microchannel with constriction and notations used here are given in Fig. 5.1. The pressure downstream and upstream of the constriction are unknowns. We will denote them $p_1$ and $p_2$ (see Fig. 5.1).

The flow quantity that has to be conserved in all three sections is the mass flow. The mass flow conservation yields a system of three non-linear algebraic equations for the unknown mass flow, $m^*$, and two unknown pressures, $p_1$ and $p_2$. The mass flow in a dimensional form for a high-aspect ratio straight microchannel for a given pressure ratio is equal to [9]:

$$
\dot{m} = \frac{H^3 dp_{out}^2}{24\mu LRT} (P - 1 + 12\alpha_r Kn_{out}(P - 1)) \quad (5.2)
$$

Applying the mass flow formula for each section, we get the system:

$$
\dot{m}(p_{in}, p_1, L_1, H_1, Kn_1) = m^* \quad (5.3)
$$

$$
\dot{m}(p_1, p_2, L_2, H_2, Kn_2) = m^* \quad (5.4)
$$

$$
\dot{m}(p_2, p_{out}, L_3, H_3, Kn_0) = m^* \quad (5.5)
$$
where $Kn_1 = Kn_{out} p_{out}/p_1$ is the Knudsen number at the location just upstream of the constriction. Similarly, $Kn_2 = Kn_{out} p_{out}/p_2 H_3/H_2$ is the Knudsen number downstream of the constriction based on the constriction height.

The non-linear algebraic system can be solved by an optimization method. The least square method was used and iterations were carried out until the agreement for mass flow up to fifth significant digit was reached.

5.3 Subsonic inlet and outlet boundary conditions for DSMC method

5.3.1 Implementation

The numerical simulation of a subsonic flow in a pressure-driven microchannel requires a special treatment of the inlet and outlet boundary conditions. If the flow is in the subsonic regime then the one-dimensional characteristic theory dictates that there will be two incoming characteristic lines along which information propagates at the inlet and one incoming characteristic line at the outlet. Therefore, only two flow parameters out of three (pressure, temperature and velocity) can be freely specified at the inlet and only one at the outlet. On the other hand, in the DSMC method all three flow parameters must be specified for incoming molecules at the domain boundaries, i.e. density, temperature and velocity. In this case, boundary conditions have to use flow properties in the interior flow domain.

The implementation of subsonic inlet and outlet boundary conditions for various computational fluid dynamics (CFD) methods has been intensively studied in the
past [87]. The DSMC method has only been relatively recently applied for such flow simulations that require an implicit subsonic boundary conditions treatment. For an inflow boundary, the most common approach is to determine streamwise velocity from the information in the interior flow domain. This was first applied by Ikegawa and Kobayashi [37] when the streamwise velocity at the inlet was computed based on total particle flux in the computational domain. Nance et al. [70] employed the particle conservation at each cell to determine the unknown streamwise velocity at the exit. Finally, several workers [71, 29] have implemented and tested a simpler approach when the unknown velocity at the inlet has been determined by extrapolation from the cell adjacent to the boundary. This treatment of inlet boundary has been adapted in the present DSMC simulations.

At the microchannel outlet the only known flow property is pressure. Therefore, temperature and velocity have to be determined from the information in the interior flow domain. A one-dimensional characteristic theory can be applied in the following way. For a backward-running wave:

\[
\frac{du}{a} = -\frac{d\rho}{\rho}\tag{5.6}\]

where \(a\) is the speed of sound, \(a^2 = \frac{dp}{d\rho}\). Applying the definition of the speed of sound in a finite difference form to a boundary cell, one obtains:

\[
\rho_e = \rho_{int} + \frac{p_e - p_{int}}{a_{int}^2}\tag{5.7}\]

thus, temperature at the outlet can be found from ideal gas law. From Eq. 5.6:

\[
u_e = \nu_{int} - \frac{p_{int} - p_e}{a_{int}\rho_{int}}\tag{5.8}\]
The above equations for determining temperature and velocity at the subsonic outlet given a pressure value are called Whitfield’s characteristic formulation [87]. In the present implementation, the Whitfield characteristic formulation was used in the cell subject to condition that the pressure in the cell is larger than the specified outlet pressure. Otherwise, extrapolation of velocity and temperature has been applied. The inlet and outlet conditions used in DSMC are updated based on the above procedure every 20,000 time steps to avoid statistical scatter in the flow macroparameters in the interior cells.

5.3.2 Validation

To validate the implementation of the subsonic boundary conditions in the DSMC method, a test case of nitrogen flow in a straight microchannel has been calculated and compared with the analytic approximate solution [9]. The microchannel aspect ratio is 30 and Knudsen number based on the outlet conditions is 0.05. The pressure ratio between inlet and outlet is 2.47. The inlet temperature of the gas is 300 K which corresponds to a value of the viscosity coefficient of $1.77 \times 10^{-5} \text{ kg/m} \cdot \text{s}$ based on the hard-sphere model with a viscosity-temperature exponent of 0.24 and molecular diameter of $4.17 \times 10^{-10} \text{ m}$. The large aspect-ratio microchannel is in the slip-flow regime and the analytic approximate solution for such flow was obtained by Arkilic et al [9].

Application of a numerical method to solve practical problems requires a reliable way to estimate the accuracy of the solution. The DSMC numerical solution depends on three parameters: the cell size $\Delta x$, time step $\Delta t$, and the number of particles $N_\lambda$ in a volume with linear size equal to the local mean free path [39]. In the DSMC algorithm, the cell size has to be less than the local mean free path and the time step should be less
than the average time between collisions. However, a more strict requirement is that the number of simulated particles has to be large enough to make the statistical correlations between particles insignificant.

The principal objective of the validation study presented below was to examine the sensitivity of the results to the above numerical parameters of the DSMC simulation and to compare the computed flow parameters with the analytic predictions.

The calculations with different time steps showed that the results do not change when $\Delta t$ is decreased from $5 \times 10^{-5}$ s to $1 \times 10^{-5}$ s. The time step of $3 \times 10^{-5}$ s was chosen for all calculations presented hereafter. The cell size was found to have a larger impact on the DSMC solution. The influence of the number of cells on the streamwise velocity profile along the axis is shown in Fig. 5.2 for 1.6 million particles. There is a difference of about 10% when the number of cells is changed from 50,000 to 100,000. The solution does not change when the number of cells is further increased to 200,000. Note that the pressure distribution is practically unaffected by the number of cells. As shown in Fig. 5.3 the maximum pressure difference amounts to less than 1%.

The most important parameter for the accuracy of the DSMC method is the number of simulated molecules. In the present validation study, the number of simulated molecules has been varied from 0.2 million to 12.8 million. Similar to the influence of the number of cells, the pressure distribution is insensitive to the variation of the number of molecules. The maximum difference between the results for 0.2 million and 12.8 million was less than 2%. The most sensitive parameter to the number of molecules is the streamwise velocity. Figure 5.4 shows that the streamwise velocity changes when the
number of molecules is less than 3.2 million. The difference between the solution for 0.2 million and 3.2 million is over 20%.

The main reason for the strong dependence of the solution on the number of particles is related to the correlations between simulated particles. Such correlations always exist in the system of a finite number of particles used in DSMC modeling [44]. The magnitude of these correlations depends on the total number of simulated molecules in the system, and generally decreases when the number of molecules increases. It is necessary to estimate the level of statistical dependence between the simulated particles and its contribution to the results of DSMC computation. A significant level of statistical dependence, or particle correlations, means that the molecular chaos hypothesis, used in the Boltzmann equation, is no longer valid.

An important criterion that allows for a practical verification of the presence of the statistical dependence between simulated particles is the relative number of repeated collisions [39]. Repeated collisions are collisions between the same pair of particles during their lifetime in the computational domain. The lifetime of a molecule in DSMC modeling is determined by the time the molecule was introduced into the computational domain or reflected from a diffuse wall and the time it left the domain or collided with a diffuse wall. The number of repeated collisions was calculated by checking if the current collision partner of a marked particle coincides to one of the last four of its collision partners.

The number of repeated collisions is closely related to the number of particles $N_\lambda$ in a volume with the linear size equal to the local mean free path. If $N_\lambda \gg 1$, one can say that the simulation results are close to the solution of the Boltzmann equation.
The number of repeated collisions may also depend on the time step and the number of particles per collision cell.

The flow under consideration is characterized by low average velocities and, as a result, relatively large particle lifetimes. The number of repeated collisions may therefore be larger than that in a typical supersonic flow with same $N_\lambda$. The results presented in Table 5.1 for the test validation case discussed above show the average number of repeated collisions for various numbers of molecules and cells. From the comparison with Figs. 5.2-5.4, it can be seen that the number of repeated collisions in this flow has to be less then 5% for the results to be accurate within 2%.

Finally, the calculated DSMC macroparameters are compared to the analytic solution for a straight microchannel flow [9]. The total number of cells in the DSMC calculation was 200,000 with about 12.8 million simulated particles. The pressure distribution along the channel is given in Fig. 5.5. The difference between the two solutions does not exceed 1%. The comparison of DSMC computed and analytic contours of X-component of velocity are plotted in Fig. 5.6 and also shows excellent agreement. All the calculations presented in the following sections were performed with the same $N_\lambda = 256$. The DSMC calculations of microchannel flows presented in this chapter were made on 260 node MHPCC Linux SuperCluster. The total CPU time for a typical calculation was about 48 hours using 32 Pentium III 933 MHz processors.

5.4 Comparison with DSMC modeling

The DSMC calculations of low-speed microchannel flows with constriction of a finite length have been carried out in order to study the influence of the constriction on
the pressure loss, mass flow rate and the overall flow structure in the channel. The results of the DSMC simulations are then compared with the simple model of constriction. The flow conditions and geometries of the microchannels are summarized in Tables 5.2 and 5.3.

5.4.1 Pressure losses

Let us first consider Case 1 which corresponds to the same total pressure loss as in the case of a straight microchannel that was used for validation of the boundary conditions. The presence of the constriction significantly changes the pressure distribution inside the channel. The pressure distribution along X-axis is plotted in Fig. 5.7 along with that for a straight channel and a theoretical prediction of Eq. (5.3)-(5.5). The DSMC calculated pressure distribution agrees very well with the theoretical prediction. The maximum difference is immediately downstream of the constriction but still is within 3% of the computed value. The pressure loss at the constriction section is about 60% of the total pressure loss and, therefore, can not be considered a “minor” loss.

Figure 5.9 shows the comparison of theoretical and simulated DSMC pressure distributions along the X-axis for the other cases given in Table 5.3. In all three cases, pressure values are in excellent agreement. Therefore, the flow in a microchannel with a constriction of finite length can be considered as three different microchannels flows and system (5.3)-(5.5) can be used to calculate the pressure loss in the constriction section.
5.4.2 Flow structure

Let us now consider the flow structure near the constriction section as predicted by the DSMC simulations. Figure 5.11 shows the pressure contours near the constriction section. There is a small adverse pressure gradient at the corners downstream and upstream of the constriction. The pressure isolines are normal to X-axis everywhere in the flow except the inlet and outlet of the constriction section where the isolines have a nearly circular shape as the flow becomes fully developed. Overall, the flow structure in the microchannel with constriction of a finite length is very well approximated by three different channel flows.

The streamlines and contours of X-component of velocity are shown in Fig. 5.10 for Case 1. Far from the constriction, the streamlines of the flow are parallel to X-axis and the value of the streamwise velocity is about 12 m/sec at the centerline.

The flow in the microchannel with constriction separates in the transition section similarly to a flow around forward and rear-ward steps. The two separation zones are clearly identified at the corners immediately upstream and downstream of the constriction section. The size of the separation zone upstream is equal to about half of the constriction height. The separation zone downstream is slightly larger due to a larger flow velocity. The velocity in the constriction section increases to approximately 60 m/sec at the centerline. Far downstream of the constriction the value of the X-component of the velocity decreases to 22 m/sec.

A similar flow structure is observed in the other computed cases. The streamlines and X-component of velocity is plotted in Figs. 5.12-5.14 for Cases 2-4. In Cases 2-4 the
size of the separation zone upstream of the constriction is less than in Case 2 due to a much lower velocity.

The flow separation observed in the four cases may be understood in terms of standard boundary layer theory. To illustrate this, Case 1 was re-run assuming a fully specular gas-surface interaction for the upstream channel. Although such a situation is physically unrealistic for microchannel flows, the simulation corresponds to one of ideal flow. In this case, no flow separation is observed and the streamlines follow the corner boundaries. Hence in the real transitional subsonic microchannel flow, recirculation will occur even for low Reynolds numbers.

5.4.3 Mass flow losses

The mass flow of in a microchannel for a specific inlet to outlet pressure ratio is an important characteristic for design of micro-devices. The mass flow of a microchannel with constriction can be significantly smaller compared to that of a straight microchannel, \( \dot{m}_{\text{un}} \), for the same pressure ratio. A monotonic decrease of the mass flow with the decreasing constriction-gap width has been observed experimentally [55].

Theoretical and calculated mass flow of a constriction microchannel divided by that of a corresponding straight microchannel is listed in Table 5.4 for Cases 1-4. Both theoretical and calculated mass flow in a constriction microchannel indicate very large mass flow losses compared to straight microchannel.

The results of the calculation agree within a few per cent with the theoretical prediction for Cases 1, 2, and 4. The maximum difference (18%) between theory and
DSMC is in Case 3, where the flow Knudsen number at the outlet is 0.1 and therefore, the slip flow approximation used in Eq. 5.3-5.5, may no longer be accurate.

5.5 Summary

The subsonic gas flow through a microchannel with a finite-length constriction is studied with the goal of predicting the significant pressure and mass flow rate losses observed in earlier experimental studies. An analytic model is proposed that allows one to predict the pressure and mass flow losses due to the constriction. The model is validated by comparison with the numerical results obtained using the direct simulation Monte Carlo method. The agreement between the predicted analytic and DSMC solutions is found to be very good with the maximum difference smaller than a few percent.

The analysis of the sensitivity of the DSMC results to numerical parameters was also conducted, and the large impact of correlations between simulated particles in the low-speed flows under consideration was shown. The DSMC results indicate that the flow in the microchannel with constriction separates in the transition section similarly to a flow around forward and rear-ward steps. However, the separation region does not significantly impact the pressure distribution along the channel.

The pressure loss in the transition section is as large as 60% and, therefore, cannot be considered a minor loss. The mass flow rate ratio between the constriction and straight channel varies from 15 to 40% for the considered cases. Therefore, the constriction has a dramatic effect on the major system design parameters for a pressure-driven microchannel flow.
Fig. 5.1. Schematic of a microchannel with constriction.

Fig. 5.2. Streamwise velocity distribution along the channel, $Kn_{out}=0.05$, $L/H=30$ for different numbers of cells.
Fig. 5.3. Normalized pressure distribution along the channel, $Kn_{out}=0.05$, $L/H=30$ for different numbers of cells.
Fig. 5.4. Streamwise velocity distribution along the channel, $Kn_{out} = 0.05$, $L/H = 30$ for different numbers of particles.
Fig. 5.5. Normalized pressure distribution along the channel, $Kn_{out}=0.05$, $L/H=30$. 
Fig. 5.6. Streamwise velocity (m/s) contours, $Kn_{out}=0.05$, $L/H=30$. Analytic solution [9]- dashed lines, DSMC solution - solid lines.
Fig. 5.7. Comparison of simulated and theoretical pressure distribution Eq. (5.3)-(5.5) for Case 1.
Fig. 5.8. Comparison of calculated and theoretical pressure distribution Eq. (5.3)-(5.5) for Case 2.
Fig. 5.9. Comparison of calculated and theoretical pressure distribution Eq. (5.3)-(5.5) for Case 3 and 4.
Fig. 5.10. X-component of velocity contours and streamlines for Case 1.
Fig. 5.11. Pressure contours for Case 1.

Fig. 5.12. X-component of velocity contours and streamlines, Case 2.
Fig. 5.13. X-component of velocity contours and streamlines, Case 3.

Fig. 5.14. X-component of velocity contours and streamlines, Case 4.
Table 5.1. Number of repeated collisions for validation test conditions (straight channel, $Kn_{out} = 0.05$, $\frac{p_{in}}{p_{out}} = 2.47$, $\frac{L}{H} = 30$).

<table>
<thead>
<tr>
<th>Number of particles, million</th>
<th>Number of cells, $10^3$</th>
<th>$N_\lambda$</th>
<th>Percentage of repeated collisions</th>
</tr>
</thead>
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<tr>
<td>0.2</td>
<td>80</td>
<td>4</td>
<td>32</td>
</tr>
<tr>
<td>0.8</td>
<td>160</td>
<td>16</td>
<td>8</td>
</tr>
<tr>
<td>1.6</td>
<td>50</td>
<td>32</td>
<td>2.5</td>
</tr>
<tr>
<td>1.6</td>
<td>100</td>
<td>32</td>
<td>3.5</td>
</tr>
<tr>
<td>1.6</td>
<td>200</td>
<td>32</td>
<td>5.0</td>
</tr>
<tr>
<td>3.2</td>
<td>200</td>
<td>64</td>
<td>3.0</td>
</tr>
<tr>
<td>6.4</td>
<td>200</td>
<td>128</td>
<td>2.5</td>
</tr>
<tr>
<td>12.8</td>
<td>200</td>
<td>256</td>
<td>2.0</td>
</tr>
</tbody>
</table>

Table 5.2. Geometric setup

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<tr>
<th>Shape</th>
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<th>$H_3/H_1$</th>
<th>$L_1/H_1$</th>
<th>$L_2/H_1$</th>
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<td>14.5</td>
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<td>14.5</td>
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<tr>
<td>2</td>
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<td>1</td>
<td>8.5</td>
<td>3</td>
<td>8.5</td>
</tr>
</tbody>
</table>

Table 5.3. Summary of cases considered

<table>
<thead>
<tr>
<th>Notation</th>
<th>$\frac{p_{in}}{p_{out}}$</th>
<th>$Kn_{out}$</th>
<th>Shape</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>2.47</td>
<td>0.05</td>
<td>1</td>
</tr>
<tr>
<td>Case 2</td>
<td>2.53</td>
<td>0.05</td>
<td>2</td>
</tr>
<tr>
<td>Case 3</td>
<td>2.47</td>
<td>0.1</td>
<td>2</td>
</tr>
<tr>
<td>Case 4</td>
<td>1.25</td>
<td>0.05</td>
<td>2</td>
</tr>
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</table>
Table 5.4. Theoretical and calculated mass flow losses

<table>
<thead>
<tr>
<th>Case</th>
<th>Theory $\dot{m}/m_{un}$, %</th>
<th>DSMC $\dot{m}/m_{un}$, %</th>
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</thead>
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</tr>
<tr>
<td>3</td>
<td>15.8</td>
<td>18.7</td>
</tr>
<tr>
<td>4</td>
<td>14.8</td>
<td>15.2</td>
</tr>
</tbody>
</table>
Chapter 6

An Application of DSMC for Micropropulsion Testing

6.1 Background and motivation

The ability to measure extremely low thrust levels with high precision is becoming more critical as attempts are made to characterize the performance of emerging micropropulsion systems. The measurement of the thrust of microscale propulsion devices, such as cold gas and mono- and bi-propellant thrusters, and resistojets, is a difficult task due to the very low thrust levels, on the order of milli- and micro-Newton. For such force levels, facility vibrations and test stand drift can lead to significant measurement errors [11, 19]. On the other hand, the accurate modeling of flows in micropropulsion systems is often hampered by the many uncertainties in the flow and material characteristics such as the distribution of wall temperature, viscosity-temperature exponents for a specific mixture, and internal energy transfer models. In this case, the orifice flow with the comparable thrust levels can serve as a calibration test for milli- and micro-Newton thrust-stands. This chapter describes the modeling and experimental results of mass flux and thrust force for nitrogen, helium and argon orifice flow at room temperature.

This chapter presents the direct simulation Monte Carlo (DSMC) calculations of orifice flow in the transitional regime with the specific goal of using the calculations for comparison with mass flux and thrust force measurements [50]. The accuracy of the DSMC simulations of a gas flow depends on two major factors: first, on the accuracy of
the molecular model used to represent the physical gas flow phenomena, and second, on the accuracy of the statistical simulation itself, \textit{i.e.} resolution in terms of the number of simulated particles, time step and cell size of the spatial mesh. For the experimental conditions considered in this work: room temperature, argon, nitrogen, and helium test gases, molecular collision parameters such as the viscosity-temperature exponents and molecular diameters are well known. Moreover, the computational requirements are easily met for the orifice flow in the Knudsen number regime from 0.01 to 40. This allows one to obtain very accurate numerical results by applying the DSMC method. The results presented in this chapter were published in parts in Ref. [3].

6.2 Orifice flow theory

The steady flow of a gas through an infinitesimally thin orifice, so called orifice flow, is a classical problem of fluid mechanics [79]. Besides the theoretical interest there are many practical applications in space environment and vacuum technology where orifice flow is important. An extensive experimental study of orifice flow has been conducted in the past. For gas expansion through an orifice the analytical solution is known for the limiting case of Knudsen number $Kn = \infty$, \textit{i.e.} a collisionless flow. The first-order corrections for the mass flux of a thin orifice were obtained by Liepmann [58] for near zero and large $Kn$. Numerical results for the mass flux in the near-free molecular regime were obtained using a first-iterate solution of the Boltzmann equation [88] and were found to agree with experimental data [58]. It is also known that in the continuum limit ($Kn = 0$) the mass flux through an orifice of negligible lip thickness is always less than that of a comparable smooth nozzle [58]. The discharge coefficient, \textit{i.e.} the ratio of the
orifice mass flux to that of an isentropic inviscid nozzle flow with the same throat area, was measured by different workers for various gases and aperture shapes at high $Re$, the specific values may be found in Ref. [60].

In the transitional regime, $Kn$ on the order of 0.01 to 10, there is no analytical solution to the orifice flow and experimental data are scarce. Non-equilibrium phenomena, such as a non-Maxwellian velocity distribution and translational-rotational non-equilibrium are important in this regime [85].

In this section, the reference formulas for mass and momentum flux related to orifice flow at zero and infinite Reynolds numbers are given [58]. The Reynolds number for orifice flow can be defined as

$$Re = \frac{\rho_0 U_0 d}{\mu}$$

where $U_0 = \sqrt{\gamma R T_0}$ is the speed of sound in the reservoir. The gas properties in the reservoir (plenum) denoted with the subscript 0 will be referred to later as plenum conditions.

6.2.1 Free molecular regime

For zero Reynolds number, i.e. in the collisionless limit where the mean free path in the stationary gas at the reservoir is much larger than the orifice diameter, the mass flux is

$$\dot{m} = \frac{1}{\sqrt{2\pi RT_0}} (p_0 - p_b) A$$  \hspace{1cm} (6.1)

and the momentum flux is

$$F = \frac{p_0 - p_b}{2} A$$  \hspace{1cm} (6.2)
6.2.2 Continuum regime

The mass flux for an orifice with a negligible lip thickness is less than that of a smooth nozzle

\[ \dot{m} = C_d \dot{m}_n \]  

(6.3)

where \( C_d = C_d(\gamma, Re) \) is the discharge coefficient of the orifice flow. A typical value of \( C_d \) for a diatomic gas is 0.85 [60].

6.3 Comparison with experiment

6.3.1 Experimental setup

The orifice has a diameter \( d = 1.0 \) mm and a thickness \( t = 0.015 \) mm and is machined in a tantalum shim attached to an aluminum plenum. The plenum is mounted on a torsional thrust stand. A schematic of the setup is shown in Fig. 6.1. The measurements of the mass flux have been made at the gas inlet with an MKS mass flow meter. The force measurements were made by sensing the angular deflection of the thrust stand arm due to the total torque force. The angular deflection was detected by measuring the linear displacement using a linear differential voltage transducer. The details on the thrust stand characteristics are reported in Refs. [50] and [82].
6.3.2 Force measurements

In ground-based low thrust measurements the influence of the facility background gas can be significant and has to be accounted for. The total force measured by the thrust stand is due to four sources as shown in Fig. 6.2:

\[ \vec{F} = \vec{F}_t + \vec{F}_j + \vec{F}_b^+ + \vec{F}_b^- \]  

(6.4)

where \( \vec{F}_t \) is the thrust force produced by the momentum flux through the orifice on the thrust stand, \( \vec{F}_j \) is the force produced by the momentum flux of the jet gas on the surface of the plenum (jet backflow), \( \vec{F}_b^+ \) and \( \vec{F}_b^- \) are the forces exerted by the facility background gas on the two opposite plenum surfaces.

6.4 Modeling approach

The SMILE code [41] based on the DSMC method is used to calculate orifice flow for vacuum and finite background pressure conditions. The majorant frequency scheme [44] of the DSMC method is utilized to model collisions between molecules. The intermolecular potential is assumed to be a variable hard sphere model [15] with the molecular parameters of Ref. [16]. The jet and background gases are modeled as distinct species in order to study the influence of the facility background conditions. Due to the large pressure ratio between the plenum and the vacuum facility (from \( 10^3 \) to \( 10^7 \)), accurate resolution of the background gas can only be obtained by using different background and jet species weights in the simulations.
Due to the symmetry of the problem, the axisymmetric version of the SMILE code has been used. The computational domain and the boundary conditions are shown in Fig. 6.3. The flow conditions for the three test gases are given in Tables 6.1-6.4. The gas flux corresponding to the given plenum and background pressure and room temperature \(T_0 = 300 \text{ K}\) is modeled on the outer boundaries of the computational domain. The full momentum and energy accommodation model was assumed at the surface with a wall temperature 300 K. The collision cell size is chosen to be less than the local molecular mean free path. The number of collision cells was varied from 10,000 to 110,000 with 150,000 to 1,200,000 modeling particles, respectively, depending on the plenum pressure.

Let us now give some details on the calculation of forces used in the DSMC simulations. The impulse flux through the orifice \(F_t\) is

\[
F_t = \int_A \rho \overrightarrow{u}^2 dA =
\]

\[
\int_A \rho \left( \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_0^{\infty} u^2 f(u,v,w) du dv dw \right) dA
\]

where \(f(u,v,w)\) is the velocity distribution function, \(\rho\) is the local gas density and \(u\) is the axial velocity component. For an equilibrium velocity distribution [16],

\[
F_t = \int_A \frac{\rho RT}{2\pi^{1/2}} \left[ se^{-s^2} + \pi^{1/2} \{1 + erf(s)\}(1/2 + s^2) \right] dA
\]

where \(s\) is the molecular speed ratio. Equation 6.6 reduces to Eq. (6.2) for a stationary gas, \(s = 0\). In the transitional flow regime, the velocity distribution function at the orifice plane is non-Maxwellian. The calculated distribution functions for the axial component
of velocity at the orifice plane are plotted in Fig. 6.4. The distribution function changes from the half-Maxwell to the local Maxwell distribution when the Knudsen number decreases from 4 \((p_0 = 0.01 \text{ torr})\) to 0.04 \((p_0 = 1 \text{ torr})\). Therefore, in the transitional regime one needs to use the DSMC simulations to calculate the thrust force given by Eq. 6.5.

The momentum fluxes on the surface of the plenum \(F_j, F_b^+, F_b^-\) are calculated from the pressure distribution over the corresponding surface as

\[
F_j = \int_{A^+} p_1 \mathrm{d}A \tag{6.7}
\]

\[
F_b^+ = \int_{A^+} p_2 \mathrm{d}A \tag{6.8}
\]

\[
F_b^- = p_b A^- \tag{6.9}
\]

where \(p_1\) and \(p_2\) are the pressure distributions on the outer plenum surface containing the orifice (see Fig. 6.3) for the jet and background gases, respectively, and \(p_b\) is the constant background pressure in the vacuum facility far from the orifice. The pressure distributions, \(p_1\) and \(p_2\), may be computed separately because the jet and background gas are treated as two distinct species. Initially, the background gas corresponds to that of a uniform background gas at \(p_b\) and \(F_b^- = F_b^+\). When flow is initiated through the orifice, the background gas is perturbed and eventually is prevented from approaching the outer surface of the plenum near the orifice, a process we will refer to as “jet-shadowing”.
6.5 Effects of the flow regime

Let us first consider the impact of the flow rarefaction on the structure of the flow in the vicinity of the orifice. The results presented in this section are for molecular nitrogen flow at two Knudsen numbers, $Kn = 0.01$ and $40$, and zero background pressure (cases 1 and 12 in Table 6.1). For the plenum pressure of 3 torr, the variation in background pressure from 0 to $6.3\times10^{-4}$ torr for the plenum pressure of 3 torr does not change the flow parameters near the orifice, where the density of the jet is several orders of magnitude higher than that of the background gas.

The pressure contours normalized by the plenum pressure are shown in Fig. 6.5 for cases 1 and 12. The flow in the vicinity of the orifice is shown here to illustrate the impact of flow rarefaction, whereas the entire computational domain was $(-5d, 30d)$ in axial direction and $(0, 30d)$ in the radial direction (see Fig. 6.3). As expected, the pressure decays more rapidly and the influence of the orifice is observed further up-stream for the more rarefied flow due to a larger mean free path. The normalized pressure at the orifice plane is about two times lower for the $Kn = 40$ case. Also, the normalized pressure for $Kn = 40$ is about two times lower than for $Kn = 0.01$ along the axis.

The flow structure for the two Knudsen numbers is different near the outer plenum wall. There is almost no collisions of jet molecules with the wall for $Kn = 40$, which is in fact a free molecular flow. Pressure isolines have therefore a near-circular shape and start at the orifice edge for $Kn = 40$. Molecular collisions in the jet for the higher pressure case cause a back flow with some jet molecules colliding with the outer wall and
then reflecting with complete energy accommodation. This results in a gradual decrease of the pressure in the direction from the orifice edge.

The impact of the wall temperature is illustrated in Fig. 6.6 where the translational temperature contours are shown. For Kn=40 case, the temperature isolines are normal to the plenum wall, whereas in the more dense case, Kn=0.01, a large temperature gradient occurs at the wall with the gas temperature rising due to gas-surface collisions. Similar to the pressure contours, the influence of the orifice propagates further downstream for \( Kn = 0.01 \).

In contrast to pressure and temperature fields, the Mach number contours are similar in the subsonic portion of the flow for the two flow regimes. The Mach number contours presented for the two Knudsen numbers in Fig. 6.7 show that the Mach number fields weakly depend on the Knudsen number in the vicinity of the orifice (up to \( M \sim 2 \)). The sonic line in both cases is located outside the plenum, while the flow at the orifice plane is subsonic in both cases.

A quantitative comparison of flow parameters across the orifice is given in Figs. 6.8 and 6.9, where the profiles of the number densities and velocities in the axial direction are shown. In those figures, \( Y/d = 0 \) corresponds to the orifice center. The profiles were taken along the cells located immediately after the orifice plane. For \( Kn = 40 \), the parameters are nearly constant up to a distance of 0.4 d from the axis. In the interval from 0.4 d to the orifice edge 0.5 d, the velocity increases and the density decreases due to the gas expansion. The shape of the density and velocity profiles is different for \( Kn = 0.01 \), where it more gradually change from the axis to the orifice edge.
6.6 Effects of the background facility gas

Consider now the effect of the jet on the flowfields and surface fluxes of the background gas. As expected, the jet molecules do not perturb the background gas for the lowest calculated plenum pressures. In this case, the flow is in free molecular regime in the whole computational domain, and the density of the background gas does not change significantly throughout the field. For higher pressures the jet significantly modifies the initially uniform background gas density. Figure 6.12 shows the number density of the background gas normalized by the number density corresponding to a background pressure of $4.2 \times 10^{-4}$ torr, and for a plenum pressure of 3 torr (Case 14, Table 6.1). It is clearly seen that the normalized density decreases from its far-field value (taken at about $25d$ downstream from the orifice) to less than 0.05 in the vicinity of the orifice. The jet flow effectively shadows the near-field of the orifice, displacing the background molecules from the region close to the outer plenum surface.

The decrease in the density of the background gas is due to collisions between jet and background molecules. Figure 6.13 shows the molecular mean free path normalized by the orifice diameter and indicates a sufficient collision rate to explain the structure seen in Fig. 6.12. Generally, the mean free path is comparable or less than the linear size of the plenum height of $30d$. Even at a distance of $20d$ from the orifice, the mean free path is about $50d$, which significantly lowers the penetration of the background molecules upstream to the surface.

The influence of the plenum pressure on the pressure distribution of the background gas along the plenum surface (the line labelled “wall” in Fig. 6.3) is shown in
Fig. 6.14. The orifice edge is located at $Y = 0$, and the surface pressure, $p_2$ of Eq. 6.8, is normalized by its value at $Y = \infty$, $p_b$. The surface pressure is almost not affected by the jet for the low-pressure case, $p_0 = 0.1$ torr. It decreases to 0.9 in the vicinity of the orifice edge, being close to unity for $Y > 5d$. For the high-pressure case, the entire area of the plenum is partially shadowed by the flow from the orifice.

The calculations were also performed for other background pressures (cases 12 through 15 in Table 6.1). An important conclusion here is that the change in the background pressure from 0 to about 0.02% of the plenum pressure does not impact the penetration of the background gas through the jet to the surface. The shadowing effect is therefore the same, and the surface pressure produced by the background gas is similar for different $p_b$ at the same plenum pressure. This is shown in Fig. 6.14 for two different background pressure values (cases 14 and 15).

To properly calculate the total force, in addition to the thrust force and the forces produced by the background, we need to include the contribution from the force produced by the orifice backflow, i.e. molecules from the jet that hit the surface. The comparison of surface pressure distributions due to jet and background gas molecules is given in Fig. 6.15 for case 14. It is seen that in the vicinity of the orifice the surface pressure produced by jet molecules is much larger than that from the background, whereas the background gas pressure is larger at $Y/d > 5$. From the pressure distributions $F_b^+$ and $F_j$ can be calculated by integrating over the plenum surface. Since the surface area for the axisymmetric case is proportional $Y^2$, the contribution to the force from background pressure, $F_b^+$ turns out to be larger than that of the jet, $F_j$, $4.4 \cdot 10^{-5}$ N and $1.76 \cdot 10^{-5}$ N, respectively.
The surface pressure from the jet increases with the background pressure, because jet-background collisions occur more frequently. This increase is close to linear, as is shown in Fig. 6.16 for cases 12-15. As was discussed above, the surface distribution of the background pressure scales linearly with the background pressure. The force produced by the background gas on the orifice side of the plenum therefore also scales linearly (Fig. 6.16). The influence of the background on the flow from the orifice is negligibly small, which results in a linear dependence of the total force on the background pressure. The computational results therefore confirm the applicability of the linear extrapolation from non-zero pressures to obtain thrust measurements for zero background pressure used in Ref. [50]. An important conclusion from Fig. 6.16 is also that the contribution from \( F_j \) and \( F_b^+ \) is larger that that from \( F_b^- \) for all background pressures under consideration.

6.7 Comparison of calculated and measured mass flux

A comparison of the calculated and measured mass flux is given in Fig. 6.10 for the nitrogen test gas cases listed in Table 6.1. The theoretical values of the mass flux for a free molecular flow (see Eq. (6.1)) and an inviscid continuum flow through an orifice with a negligible lip thickness (see Eq. (6.3)) are also shown here. A discharge coefficient of 0.86 for the continuum flow obtained in the previous work [50] is used here. The calculated mass flux for the two lowest pressure values (\( Kn = 40 \) and 4) are nearly identical to the free molecular value. Calculated mass flux approaches the continuum values as the pressure is increased. The agreement between the calculated and measured mass fluxes for pressures higher than 0.5 torr is within 2%. The agreement is worse for the lowest pressures values, due to a greater experimental errors of approximately
14% for \( p_0 = 0.1 \) torr and 3.5% for \( p_0 = 0.25 \) torr. The comparison of calculated and measured mass fluxes for Argon is given in Fig. 6.11. The similar agreement was obtained for the helium gases.

### 6.8 Thrust stand calibration using DSMC modeling

The force has been measured in the experiment by the torsional thrust stand in terms of a deflection sensed by a transducer [50, 82]. A calibration of the thrust stand has been carried out by the least square fit of the deflection data and the DSMC simulation results for \( N_2 \), He, and Ar. The calibration factor was determined to be \( 2.2 \times 10^{-3} \) N/Volts. Figures 6.17-6.19 show the comparison of calculated forces with the calibrated measured force for the three test gases. Since the orifice flow test is easy to set-up and the gases under consideration are readily available, the mass flux and thrust data presented in this chapter can be used as reference for testing micro-Newton thrust stands.

### 6.9 Summary

The direct simulation Monte Carlo method was applied to the modeling of a rarefied gas expansion through a thin circular orifice. The calculations were conducted for orifice flows for \( Kn = 0.01 \) to 40. The numerical and earlier obtained experimental results were used to calibrate a torsional thrust stand designed to measure force levels of \( 10^{-6} \) to \( 10^{-3} \) N.

For the nitrogen test gas, the calculated and measured mass fluxes agree within 5% for Knudsen number less than 0.1. The maximum deviation between the calibrated measured and calculated force is 23% for \( Kn=0.4 \) and is less than 3% for \( Kn \) less than
0.1. For the other two gases, argon and helium, data were obtained for lower background pressures, resulting in even better agreement between measurements and calculations.

The calculations have been made for different facility background pressures, with the background-to-plenum pressure ratio changed from 0 to $10^{-3}$. For low Knudsen numbers the background gas contribution to the total force becomes significant. This is due to the jet shadowing effect which is sufficiently significant and must be included in modeling to permit a comparison with experiment. The increase of the background gas force on the plenum side was found to be a linear function of background pressure.

The force contribution of the momentum flux from the jet on the plenum surface was shown to be important for lower Knudsen numbers. It is comparable to the background gas contribution for $\text{Kn}=0.01$. For the considered flow conditions, the jet backflow contribution linearly increases with background pressure. The total force depends therefore linearly on the facility background pressure. Hence, the computational results confirm the applicability of the linear assumption utilized in the experiments to extrapolate the results for zero background pressure. These calculations support the use of ground-based facilities to make reliable low thrust measurements.
Fig. 6.1. Schematic of experimental geometry.

Table 6.1. Reservoir and facility background conditions for Nitrogen.

<table>
<thead>
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<th>Case</th>
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<th>$p_b$, torr</th>
</tr>
</thead>
<tbody>
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<td>1</td>
<td>40</td>
<td>0.001</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>0.01</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>0.4</td>
<td>0.1</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>0.4</td>
<td>0.1</td>
<td>$1 \cdot 10^{-4}$</td>
</tr>
<tr>
<td>5</td>
<td>0.16</td>
<td>0.25</td>
<td>$1.3 \cdot 10^{-4}$</td>
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<td>7</td>
<td>0.053</td>
<td>0.75</td>
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<td>8</td>
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<td>1.0</td>
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<td>0.026</td>
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<td>0.016</td>
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<td>$3.7 \cdot 10^{-4}$</td>
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Table 6.2. Calculated forces for Nitrogen.

<table>
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<th>$F_{h}^{-}$, $\mu$N</th>
<th>$F_{h}^{+}$, $\mu$N</th>
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Table 6.3. Conditions and calculated force for Argon.

<table>
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<th>$F$, $\mu$N</th>
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Table 6.4. Conditions and calculated force for Helium.

<table>
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Fig. 6.2. Force diagram. The density isolines are shown schematically.
Fig. 6.3. Computational domain and boundary conditions.

Fig. 6.4. Distribution function of axial velocity component at the center of the orifice.
Fig. 6.5. Normalized pressure for Kn=40 (top) and Kn=0.01 (bottom).

Fig. 6.6. Translational temperature for Kn=40 (top) and Kn=0.01 (bottom).
Fig. 6.7. Mach number for Kn=40 (top) and Kn=0.01 (bottom).

Fig. 6.8. Density and velocity profiles at the orifice plane for Kn=40
Fig. 6.9. Density and velocity profiles at the orifice plane for Kn=0.01

Fig. 6.10. Mass flux vs plenum pressure for Nitrogen.
Fig. 6.11. Mass flux vs plenum pressure for Argon.

Fig. 6.12. Normalized density of background gas for Case 14.
Fig. 6.13. Local mean free path normalized by the orifice diameter for Case 14.
Fig. 6.14. Normalized pressure distribution of the background gas along the plenum wall.
Fig. 6.15. Pressure distribution along the plenum wall.
Fig. 6.16. Different forces as function of the background pressure.

Fig. 6.17. Measured and calculated total force for Nitrogen.
Fig. 6.18. Measured and calculated total force for Argon.

Fig. 6.19. Measured and calculated total force for Helium.
Chapter 7

Conclusions

The research conducted for this thesis was the numerical modeling of microscale gas flows using direct simulation Monte Carlo method. The objectives were to improve physical understanding of gas flow phenomena important in Micro-Electro-Mechanical Systems, develop numerical approach for accurate modeling of such flows, establish validity by direct comparisons with experimental measurements, and apply it to investigate the challenging problems involving gaseous flows in MEMS.

The investigation of physical processes in three-dimensional micronozzle flows and the influence of Reynolds number, geometrical configuration and temperature regime was carried out in the thesis. The comparison of the DSMC and Navier-Stokes solutions for cold gas micronozzle flow showed a satisfactory agreement for the flow inside the nozzle. There is a significant difference between them in the nozzle lip region. The use of an external zone in the continuum approach, which starts at the nozzle exit and expands downstream, allows one to eliminate the possible impact of the extrapolation outflow boundary condition at the nozzle exit. This results in thrust values that are in agreement with those obtained using the DSMC method. The impact of wall effects on thrust level was examined for axisymmetric and two- and three-dimensional cold gas micronozzles. The flow in a flat micronozzle has a three-dimensional structure and is strongly influenced by the end walls. The additional friction losses on the side walls
cause a significant reduction in thrust (about 20%) as compared to the two-dimensional model and axisymmetric nozzle. Attempts to predict the performance characteristics of a three-dimensional microthruster using a two-dimensional model may, therefore, result in significant design errors.

The research on coupled analysis of microthruster conducted in the thesis was successful in reaching the objective of developing a numerical simulation code capable of modeling the temporal variation of microthruster material temperature and performance characteristics. The application of the developed approach to two-dimensional and three-dimensional microthrusters gave several important insights into the dependence of performance characteristics on Reynolds number, thermal conditions and thruster geometry. It was found that the mass discharge of the thruster may decrease significantly in time due to increasing wall temperature. Such behavior of the mass discharge coefficient was obtained for both 2D and 3D models as well as for different stagnation pressures and geometrical shapes.

Investigation of gas flows in microchannels with constriction was carried out both analytically and numerically in order to understand the flow phenomena observed in experiments. An analytic model was developed to predict pressure drop and mass flow rate. The validation of the model was conducted by comparison with two-dimensional DSMC calculations. It was found that the model predicts accurately the mass flow rate and pressure drop at the constriction section. The DSMC simulations have also shown that the flow separation may occur in the sharp corners of the constriction sections. The presence of the separation does not influence the pressure distribution and the mass flow rate.
The DSMC method was applied for calibration of micro-Newton thrust stand and investigation of effects of facility background. The DSMC calculations were conducted for orifice flow for $Kn = 0.01$ to $40$. It was found that for low Knudsen numbers the background gas contribution to the total force becomes significant. This was attributed to the jet shadowing effect, and, therefore, it must be included in modeling to permit a comparison with experiment. The increase of the background gas force on the plenum side was found to be a linear function of background pressure. The force contribution of the momentum flux from the jet on the plenum surface was shown to be important for lower Knudsen numbers. It is comparable to the background gas contribution for $Kn=0.01$. For the considered flow conditions, the jet backflow contribution linearly increases with background pressure. Hence, the computational results confirmed the applicability of the linear assumption utilized in the experiments to extrapolate the results to a zero background pressure. These calculations support the use of ground-based facilities to make reliable low thrust measurements.
References


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AWARDS/PROFESSIONAL ACTIVITIES
Referee, Journal of Thermophysics and Heat Transfer
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REFEREED PUBLICATIONS