International Communications in Heat and Mass Transfer 36 (2009) 402–411

Contents lists available at ScienceDirect

International Communications in Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ichmt

Size and expansion ratio analysis of micro nozzle gas flow ☆

Omer San [a], Ilhan Bayraktar [b], Tuba Bayraktar [c,*]

[a] Old Dominion University, Aerospace Eng. Dept., Norfolk, VA 23529, United States
[b] KosKom Technologies LLC, Menasha, WI 54952, United States
[c] University of Wisconsin - Platteville, Mechanical and Industrial Engineering Department, Menasha, WI 54942, United States

ARTICLE INFO

Available online 17 March 2009

Keywords:
Micro nozzle
Burnett equations
MEMS (Micro Electro-Mechanical Systems)

ABSTRACT

Size and expansion ratio effects on the flowfield are investigated for micro converging-diverging nozzles. Numerical computations are conducted by using two dimensional augmented Burnett equations and Navier-Stokes equations that were derived from the Boltzmann equation. The Maxwell-Smoluchowski slip boundary condition is used for adiabatic walls, and Steger-Warming flux vector splitting scheme is applied to the convective inviscid flux terms. The results from the augmented Burnett equation are compared with Navier-Stokes and Direct Simulation Monte Carlo (DSMC) results. Then, nozzle-size analysis is conducted for between 2 μm and 100 μm throat width. Influence of the Knudsen number is investigated, and temperature and Mach number variations are presented. In addition, the influence of the expansion ratio is studied with three (1.7:1, 3.4:1, and 6.8:1) different configurations. The results are compared with each other and an experimental data in the literature.

1. Introduction

Recent developments in micro electrical mechanical systems (MEMS) have guided the construction of many small-sized devices. Aerospace industry has benefited from these devices particularly in development of new micro-size spacecraft and satellites. However, design and development of such products have brought new challenges especially related to the aero-propulsion area. Micro nozzle flow is one of the key topics in the aero-propulsion development that needs to be studied to design the next generation micro-size aerospace vehicles.

The objective of the present study comes from the effort in simulating the flowfield and heat transfer characteristics in MEMS using computational fluid dynamics (CFD) techniques. The common CFD codes, which have been developed from Navier Stokes equation becomes especially inaccurate for microfluidic flows, because the local Knudsen number (Kn) lies beyond the continuum regime [1]. Similar challenges of such flowfield problems are also presented in the recent literature [2–5]. Typically, a flowfield with $Kn \leq 0.001$ is called as the continuum regime. The continuum-transition regime or slip flow regime is $0.001 \leq Kn \leq 0.1$, and the transition regime is between Knudsen number of 0.1 and 10. The flowfield with higher Knudsen number than 10 is generally identified as the free molecular flow. The gas flow in micro scale devices is usually categorized in the continuum-transition regime, which is neither completely in the continuum regime nor in the rarefied (free molecular flow) regime [6], and the flowfield in the nano scale devices is categorized in the transition regime [7]. Along with the direct simulation Monte Carlo (DSMC) approach, several extended numerical models have been recently introduced to model the flowfield in continuum-transition regime. Since statistical DSMC methods solve directly the Boltzmann equations with very high computational costs, more efficient numerical methods got additional consideration in the MEMS field. One of these methods is the Burnett equations that are obtained from Chapman-Enskog expansion of the Boltzmann equations with the parameter of Knudsen number [8]. There are various Burnett approximations in the literature such as conventional Burnett equations, augmented Burnett equations and BGK-Burnett equations [9,10].

Performance analysis for micro nozzle flow has become more important with the development of micro aero-propulsion systems. First experimental study on small-scale nozzle performance was performed by Rothe [11] with throat of 2.5–5 mm nozzle and a chamber pressure less than 1 atm, where the Reynolds number was in range between 55 and 550. The subsonic and supersonic parts of the Rothe's nozzle are cones with half angle of 30 and 20°, respectively, with longitudinal radius of curvature of the throat equal half of the throat radius. The test gas in experiment was nitrogen at the temperature of 300 K. Later several authors simulated the Rothe nozzle by using both the continuum based Navier Stokes equations [12,13] and the statistical based DSMC methods [14]. Rae [12] indicated that viscous boundary layer fills the nozzle for small divergence angle at low Reynolds numbers and there is a transition

☆ Communicated by W.J. Minkowycz.

* Corresponding author.
E-mail addresses: osanx001@odu.edu (O. San), ibayrakt@koskom.com (I. Bayraktar), bayraktart@uwplatt.edu (T. Bayraktar).

0735-1933/$ – see front matter © 2009 Elsevier Ltd. All rights reserved.
doi:10.1016/j.icheatmasstransfer.2009.01.021

without shock. This is accomplished by a thermalization of the flow energy. Kim [13] developed a finite volume code using the complete forms of Navier Stokes equations. He stated the trade-off between viscous losses due to the merging boundary layers and the divergence losses due to the radial component of thrust nulling with its symmetric counterpart. However, these continuum based studies did not consider the slip wall velocity effects. An experimental micro nozzle analysis with throat of 650 μm was investigated by Grisnik *et al.* [15], and Zelesnik et al. [16] compared their results obtained from direct simulation Monte Carlo methods with Grisnik's experiment. They stated that boundary layer growth can result in a significant viscous dissipation and raise the temperature of the flow expander. Further investigations of the viscous effects in supersonic MEMS-fabricated micro nozzles with minimum throat widths averaging 19 μm and 35 μm have been performed by Bait and Breuer demonstrating the capability of fabricating and testing cold gas micro nozzle [17]. Later, Liou et al. [18] studied a rectangular cross-section convergent–divergent micro nozzle with throat width of 20 μm, depth of 120 μm and the expansion area ratio of 1.7:1, which is one of the ratios studied in the present study. However, Liou *et al.* performed the numerical section of the study using two dimensional compressible Navier Stokes equations.

In the present study, the differences between Navier Stokes equations and augmented Burnett equations are analyzed, slip and no-slip boundary conditions are studied. Size and expansion ratio effects are investigated by computing both sets of equations in convergent divergent nozzles. In order to analyze the flow behavior for micro scale gas flows in wide range of nozzles several different geometries are selected. The throat width for the numerical simulations changes between 2 μm and 20 μm, and expansion ratio ($ER = D_e$: D_t) is between 1.7:1 and 6.8:1. Different outlet pressure boundary conditions are applied while the inlet pressure is kept at 100 kPa. Based on the case, the upper and lower boundaries are modeled as slip or non-slip walls.

2. Governing equations

The two dimensional, augmented Burnett equations written in a generalized curvilinear coordinate system (ξ, η) can be expressed in a strong conservation form as;

$$\frac{\partial \tilde{Q}}{\partial \tau} + \frac{\partial \tilde{E}_1}{\partial \xi} + \frac{\partial \tilde{F}_1}{\partial \eta} = \frac{\partial \tilde{E}_V}{\partial \xi} + \frac{\partial \tilde{F}_V}{\partial \eta} \tag{1}$$

where,

$$\begin{aligned} \tilde{Q} &= Q/J \\ \tilde{E} &= \left(\xi_x E + \xi_y F\right)/J \\ \tilde{F} &= \left(\eta_x E + \eta_y F\right)/J \\ \tilde{E}_V &= \left(\xi_x E_V + \xi_y F_V\right)/J \\ \tilde{F}_V &= \left(\eta_x E_V + \eta_y F_V\right)/J \end{aligned}$$

where J represents the transformation Jacobian and, Q is the conservative variables flux term, E_I and F_I are the inviscid-flux vector terms and E_V and F_V are the viscous-flux vector terms given as follows;

$$Q = \begin{Bmatrix} \rho \\ \rho u \\ \rho v \\ \rho e_t \end{Bmatrix} \quad E_I = \begin{Bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (\rho e_t + p)u \end{Bmatrix} \quad E_V = \begin{Bmatrix} 0 \\ \sigma_{11} \\ \sigma_{12} \\ \sigma_{11}u + \sigma_{12}v - q_1 \end{Bmatrix}.$$
$$F_I = \begin{Bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (\rho e_t + p)v \end{Bmatrix} \quad F_V = \begin{Bmatrix} 0 \\ \sigma_{21} \\ \sigma_{22} \\ \sigma_{21}u + \sigma_{22}v - q_2 \end{Bmatrix} \tag{2}$$

The constitutive equations for a gas flow near thermodynamic equilibrium can be derived as approximate solutions of the Boltzmann equation using the Chapman-Enskog expansion. This method yields the general constitutive relations for the stress tensor σ_{ij} and the heat-flux vector q_i as follows;

$$\sigma_{ij} = \sigma_{ij}^{(0)} + \sigma_{ij}^{(1)} + \sigma_{ij}^{(2)} + \cdots\cdots\cdots + \sigma_{ij}^{(n)} + O\left(Kn^{n+1}\right) \tag{3}$$

$$q_i = q_i^{(0)} + q_i^{(1)} + q_i^{(2)} + \cdots\cdots\cdots + q_i^{(n)} + O\left(Kn^{n+1}\right) \tag{4}$$

where n represents the order of accuracy with respect to Kn number which is defined as;

$$Kn = \frac{\lambda}{L} \tag{5}$$

where L is the macroscopic characteristic length, and the mean free path λ is given by:

$$\lambda = \frac{16\mu}{5\rho\sqrt{2\pi RT}}. \tag{6}$$

In case of $Kn \approx 0$, only the first terms in Eqs. (3) and (4) are considered. The zeroth-order approximation $(n=0)$ results in the Euler equations with $\sigma_{ij}^{(0)} = 0$ and $q_i^{(0)} = 0$. With the increasing Kn number the other terms in Eqs. (3) and (4) become important for the accurate representation of the stress and the heat transfer properties of the gas flow. The first order approximation represents the Navier-Stokes equations for the continuum and early transition regime with molecular diffusion. The first order stress tensor and the heat flux terms $(n=1)$ are given as;

$$\sigma_{11}^{(1)} = \mu\left(\delta_1 u_x - \delta_2 v_y\right) \tag{7}$$

$$\sigma_{12}^{(1)} = \sigma_{21}^{(1)} = \mu\left(u_y + v_x\right) \tag{8}$$

$$\sigma_{22}^{(1)} = \mu\left(\delta_1 v_y - \delta_2 u_x\right) \tag{9}$$

$$q_1^{(1)} = -\kappa T_x \tag{10}$$

$$q_2^{(1)} = -\kappa T_y. \tag{11}$$

The coefficients (δ_1, δ_2) are $(4/3, 2/3)$. As Kn becomes larger in continuum transition and early transition flow regimes, additional higher order terms in Eq. (2) are required. The second-order approximation yields the conventional Burnett equations that retain the first terms in Eq. (2). The expression for stress and heat-flux terms $(n=2)$ are obtained as;

$$\begin{aligned} \sigma_{11}^{(2)} = -\frac{\mu^2}{p}(&\alpha_1 u_x^2 + \alpha_2 u_x v_y + \alpha_3 v_y^2 + \alpha_4 u_x v_y + \alpha_5 u_y^2 + \alpha_6 v_x^2 \\ &+ \alpha_7 RT_{xx} + \alpha_8 RT_{yy} + \alpha_9 \frac{RT}{\rho}\rho_{xx} + \alpha_{10}\frac{RT}{\rho}\rho_{yy} + \alpha_{11}\frac{RT}{\rho^2}\rho_x^2 \\ &+ \alpha_{12}\frac{R}{\rho}T_x\rho_x + \alpha_{13}\frac{R}{T}T_x^2 + \alpha_{14}\frac{RT}{\rho^2}\rho_y^2 + \alpha_{15}\frac{R}{\rho}T_y\rho_y + \alpha_{16}\frac{R}{T}T_y^2) \end{aligned} \tag{12}$$

$$\begin{aligned} \sigma_{22}^{(2)} = -\frac{\mu^2}{p}(&\alpha_1 v_y^2 + \alpha_2 u_x v_y + \alpha_3 u_x^2 + \alpha_4 u_y v_x + \alpha_5 v_x^2 + \alpha_6 u_y^2 \\ &+ \alpha_7 RT_{yy} + \alpha_8 RT_{xx} + \alpha_9 \frac{RT}{\rho}\rho_{yy} + \alpha_{10}\frac{RT}{\rho}\rho_{xx} + \alpha_{11}\frac{RT}{\rho^2}\rho_y^2 \\ &+ \alpha_{12}\frac{R}{\rho}T_y\rho_y + \alpha_{13}\frac{R}{T}T_y^2 + \alpha_{14}\frac{RT}{\rho^2}\rho_x^2 + \alpha_{15}\frac{R}{\rho}T_x\rho_x + \alpha_{16}\frac{R}{T}T_x^2) \end{aligned} \tag{13}$$