Numerical study of micro-scale gas flow using finite volume method

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Abstract. Numerical studies of subsonic gas flow through micro-thruster as no-slip benchmark problem and high speed gas flow through short micro-channel with slip and temperature jump correction have been carried out by solving two dimensional compressible Navier-Stokes (NS) system of equations. A 2-D explicit finite volume (FV) flow solver has been developed using modified advection upwind splitting methods (AUSM+) to achieve the solution of micro-scale gas flow having high resolution shock capturing ability. The results obtained are compared with published 1-D numerical, Direct Simulation Monte Carlo (DSMC) and 2-D Finite element (FEM) results. This study utilizes the robustness and accuracy of AUSM+ and FVM to predict the micro-scale gas flows with simple explicit time marching, ranging from subsonic to supersonic flow.

1. Introduction

Microelectromechanical systems (MEMS) refer to devices that have typical characteristic lengths lying between 1 micron and 1 mm that combine electrical and mechanical components and are fabricated using integrated circuit batch processing technologies [1]. Micro-ducts, micro-pumps, micro-turbines, micro-reactors, micro-spacecraft and micro-valves are examples of small devices involving the flow of liquids and gases [2]. Usually MEMS devices work in gaseous environment under standard atmospheric conditions [3]. Since surface to volume ratio of micro-structures is very high, surface effects dominates over volumetric effects. The local Knudsen number ($Kn$) is a measure of the degree of rarefaction of gases encountered in MEMS devices.

The popular methods for analyzing the heat transfer characteristics of gases in micro-channels include the particulate method of Boltzmann equations, DSMC and Burnett equation models [4]. Several investigators have used the DSMC approach especially in case of high-speed flows, where the Knudsen number is very high, involving high computation cost and time requirement. Silicon micro-machined solid propellant based converging-diverging micro-thruster nozzle, manufactured at LAAS-CNRS, is modeled for high temperature application using no-slip continuum as a first case study. In this paper, the no-slip benchmark solutions are obtained using the indigenously developed 2-D compressible flow solver with explicit FVM using modified advection upwind splitting methods (AUSM+). The computed solutions are compared with the reported 1-D numerical results of Rossi et.al [5] and 2-D FEM results of Raju et.al [6]. This paper also aims to investigate the heat transfer characteristics of high speed compressible flow through small micro channel as a second case study. The computed results are compared with reported DSMC and 2-D FEM results [4].

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2. Problem description

The geometry of the micro-thruster chosen for analysis is taken from Rossi et al. [5] as no-slip benchmark problem. Fig.1 represents the micro-thruster that utilizes a glycidyle azide polymer (GAP) based propellant developed by the French researchers at LAAS-CNRS operating at subsonic speed. The properties of the combustion gas entering the converging-diverging nozzle are taken from Rossi et al. [5].

The working fluid for the second test case is Nitrogen gas (viscosity, \( \mu = 1.85 \times 10^{-5} \) Ns/m² and thermal conductivity, \( \kappa = 0.0259 \) W/mK) with inlet Knudsen number 0.062 through a micro-channel. The micro-channel dimensions with flow parameters are taken from Raju et al. [4]. The free stream region B (Fig. 2) is specified near the inlet section of the micro-channel where the free gas flow takes place as stated in [4].

3. Numerical methods

Finite volume discretization of the Navier-Stokes system of equations yields a set of algebraic equations that can be solved either by explicit or implicit method. Body fitted structured grids have been generated using algebraic mapping with boundary refinement to solve the discretized equations. To achieve the solutions 40×20 and 40×12 cells have been generated for micro-thruster and micro-channel respectively.

3.1. Treatment of convective flux and pressure terms

The convective terms can be considered as passive scalar quantities convected by a suitably defined velocity at the cell interface. On the other hand, pressure flux terms are governed by the acoustic wave speeds [8]. The numerical flux at a cell interface for AUSM+ with appropriate numerical speed of sound is given in [9]. The equations are as follows:

\[
F_{1/2}^{AUSM+} = \left( \begin{array}{c}
M_L^{1/8} + M_R^{1/8} \\
\beta L \end{array} \right) c_L \Psi_L + \left( \begin{array}{c}
P_L^{1/16} + P_R^{1/16} \\
\beta R \end{array} \right) c_R
\]

(1)
if \( M_{\frac{1}{2}} = M_L^* + M_R^* > 0 \), where \( \Psi = (\rho, \rho v_y, \rho v_z, \rho H)^T \) and \( P = (0, P_L^*, P_R^*, 0)^T \). The subscript \((1/2)\) stands for a quantity at a cell interface and \((L, R)\) stands for a quantity at the left and right states across a cell interface.

### 3.2. Treatment of diffusive flux and source term

The diffusive fluxes are calculated using central-average representations at the interface. The source terms for momentum and energy equations are function of viscosity and velocity gradients. These are calculated by the product of the mean value of the integrand at the control volume (CV) centre and volume of the CV.

### 3.3. Treatment of time integral: Explicit scheme

The explicit discretization using first order Euler method yields

\[
\Phi^{n+1} = \Phi^n + \int_{t_n}^{t_{n+1}} \dot{\Phi^n} dt
\]

where superscript “n” denotes the time level of iteration. The code utilizes time step dictated by Courant-Fredlich-Levy condition. The fractional change of momentum in main flow direction (y-axis) between two successive time steps is taken as the measure of convergence.

### 3.4. Boundary condition

For the first case, continuum approach has been used with no-slip wall boundary condition. The zero gradients for pressure and temperature are applied at the wall boundary. The temperature and velocity at the inlet of the nozzle are specified and the outlet pressure is also kept fixed in this case. The inlet pressure is obtained as a part of the solution. On the other hand for micro-channel at the inlet boundary, all variables are specified and their zero gradients are assumed at the outlet boundary.

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Fig. 1. Velocity (y-component) contour

Fig. 2. Temperature contour.
The first order slip condition can be written using the definition of the Knudsen number $Kn = \frac{16\mu}{\sqrt{2\pi\rho RT}}$ (based on Chapman-Enskog result [4]) as:

$$-\mu \frac{\partial v_z}{\partial z} \bigg|_{w} = \frac{5\rho \sigma_v \sqrt{2\pi RT}}{16(2-\sigma_v)} \left[ (u_{wall} - u_g) + \left( \frac{3\mu}{4\rho T_g} \right) \frac{\partial T}{\partial y} \right]$$

(3)

$$-k \frac{\partial T}{\partial z} \bigg|_{w} = \frac{\sigma_T \sqrt{2\pi RT}}{(2-\sigma_T)\left( \frac{\gamma+1}{2\gamma} \right) \frac{5\rho C_p}{16}} \left( T_{wall} - T_g \right)$$

(4)

where $\rho$ and $\mu$ are fluid density and viscosity respectively. Subscripts ‘g’ and ‘wall’ stand for properties adjacent to the wall and at the wall respectively. The tangential momentum accommodation coefficient $\sigma_v$ and the thermal accommodation coefficient $\sigma_T$ at the walls indicate the molecular fraction reflected diffusively from the walls. The slip boundary condition and temperature correction in Eq. (3) and Eq. (4) are properly applied in momentum and energy equation in this case. Near the entrance at the wall boundary for the length B (free stream region) [4], the accommodation coefficients are specified as $\sigma_v = \sigma_T = 0$. In the rest of the domain, the gas-to-wall interactions are set with $\sigma_v = \sigma_T = 1$.

4. Results and discussions

The velocity and temperature contour plots for micro-thruster problem are shown in Fig 1-2. The velocity contour plot (Fig 1.) clearly reveals the 2-D features of the fluid flow through the converging-diverging nozzle. The maximum centerline velocity appeared at the throat nearly equals to 450 m/s, showing a peak similar to that reported by Rossi et al. [5] and 2-D FEM results by Raju et al. [6]. Although the exit centerline velocity obtained by the solution is around 325 m/s as shown in Fig. 3, the average exit velocity is close to 158 m/s, which is also in accordance with the results mentioned. The Fig.2 shows that the centerline temperature is lying between 1800-1750 K. The exit centerline temperature is around 1772 K although a gradual decrease in temperature was reported by Raju et al. [6] assuming exit temperature 1700 K. The exit centerline temperature is around 1772 K although a gradual decrease in temperature was reported by Raju et al. [6] assuming exit temperature 1700 K. The pressure drop at the throat as shown in Fig. 4 also corresponds to the increase in velocity at the throat. The resulting inlet pressure is approximately 1.4 atm, which is in between the prediction reported by Raju et al. [6] and Rossi et al. [5]. The variation of centerline pressure throughout the nozzle is similar to 1-D numerical result of Rossi et al. [5]. The flow remains subsonic throughout the nozzle having the maximum Mach number close to 0.52 at the throat. The thrust predicted by the code is 20.5mN, which is 13% lower than the 1-D prediction (23 mN) by Rossi et al. [5], Raju et al. [6] reported a 44% higher prediction for the same.

For the second case the streaming velocity remains constant in ‘lighter’ region B and decreases downstream. The smooth drop in Mach number is shown in Fig. 5. The solution predicts the gradual decrease of centerline Mach to attain the value close to 1.25 at the exit, which is comparatively lower than that predicted by Raju & Roy [4]. On the other hand, the near wall Mach distribution shown in Fig. 5 is well in agreement with the prediction of Raju & Roy [4]. The code predicts higher temperature distribution compared to the reported FEM results by Raju & Roy, and DSMC results by Oh et al. [4]. The centerline and near wall temperature distributions are shown in Fig. 6. The rise in near wall temperature close to the inlet section is in accordance with the prediction of DSMC by Oh et al. [4], although the peak is higher comparatively. The downstream near wall temperature shows better matching with both DSMC and FEM results. The centre line temperature distribution obtained by the code remains higher throughout the channel.
Fig. 3. Centre line axial velocity (y–component) distribution.

Fig. 4. Centre line pressure distribution.

Fig. 5. Centerline and near wall Mach number.

Fig. 6. Centerline and near wall temperature.

5. Conclusion
A 2-D explicit finite volume flow solver has been developed using modified advection upwind splitting methods to study the micro-scale flow. 2-D compressible NS system of equations with slip/no-slip boundary condition is utilized to investigate two test cases. The numerical results for flow through micro-thruster are compared with published 1-D numerical study by Rossi et al. [5] and 2D FEM results by Raju & Roy [6] as a no-slip benchmark problem. The code predicts the essential 2-D features of the fluid flow inside the micro nozzle. The thrust calculated are comparable with that found in the literature. The first order slip boundary conditions have been successfully implemented to study the fluid flow and heat transfer characteristics in micro-channel with inlet Knudsen number 0.062 and the results are compared with the reported DSMC results by Oh et al. [4] and 2-D FEM solution by Raju & Roy [4], since no experimental data are available for this case. The code predicts higher temperature distribution and lower exit Mach comparatively. However the trends of the distributions are closely similar to DSMC results with a higher prediction.

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References

[1] Gad-el-Hak M 1999 The fluid mechanics of microdevices –The Freeman scholar lecture, J. Fluids Eng. 121 5-33.

[2] Zhang K, Chou S K and Simon S A 2004 MEMS-based solid propellant microthruster design, simulation, fabrication and testing, J. MEMS. 13 165-175.

[3] Dai J et al. 2000 Navier-Stokes simulations of gas flow in micro devices, J. Micromech. Microeng. 10 372-379.

[4] Raju R and Roy S 2005 Hydrodynamic study of high-speed flow and heat transfer through a microchannel, J. Thermophysics and Heat transfer. 19 106-113.

[5] Rossi C, Rouhani M D and Esteve D 2000 Prediction of the performance of a Si-micromachined microthruster by computing the subsonic gas flow inside the thruster, Sensors and Actuators, Physical A, 87 96-104.

[6] Raju R, Pandey B P and Roy S 2002 Finite element model of fluid flow inside a micro-thruster, Nano tech 2002-“At the edge of revolution”, Houston, Texas, AIAA-2002-5733.

[7] McNenly M J, Gallis M A and Boyd I D 2003 Slip model performance for micro-scale gas flows, Proc. 36th AIAA Thermophysics Conf. (Orlando, Florida), AIAA 2003-4050 pp. 1-9.

[8] Liou M S and Steffen C J (Jr.) 1993 A New Flux Splitting Scheme, J. of Comp. Phys., 107 23-39.

[9] Liou M S 1996 A Sequel to AUSM: AUSM+, J. Comp. Phys., 129 364-382.