Numerical Prediction of the Flow Characteristics of a Micro Shock Tube

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ABSTRACT

Recently, micro shock tube is being extensively used in various fields of engineering applications. The flow characteristics occurring in the micro shock tube may be significantly different from that of conventional macro shock tube due to very low Reynolds number and Knudsen number effects which are, in general, manifested in such flows of rarefied gas, solid-gas two-phase, etc. In these situations, Navier-Stokes equations cannot properly predict the micro shock tube flow. In the present study, a two-dimensional CFD method has been applied to simulate the micro shock tube with slip velocity and temperature jump boundary conditions. The effects of wall thermal conditions on the unsteady flow in the micro shock tube were also investigated. The unsteady behaviors of shock wave and contact discontinuity were, in detail, analyzed. The results obtained show much more attenuation of shock wave, compared with macro-shock tubes.

Key Words: Micro Shock Tube, Shock Wave, Unsteady Flow, Supersonic Flow, Slip Wall Boundary.

1. INTRODUCTION

The unsteady flow evolution and shock movement inside macro shock tubes have been widely investigated in the past. Recently with the development of MEMS and the related technologies, the study of flow physics in micro scale devices is of growing importance. Micro shock tube is one of the most extensively used devices in engineering MEMS applications. It is largely composed of the driver section and driven section which are separated by a diaphragm or a quickly opening valve. Sudden rupture of the diaphragm initiates unsteady flow from the driven section at high pressure to the driven section at a relatively low pressure. The resulting shock wave and contact surface excursions, in the case of macro tube, are very well known. Shock waves in micro tubes are used for micro heat engines for faster generation of heat. The propagation and strength of the shock waves moving inside micro devices reveals considerable deviation from that of macro tubes due to the effect of dissipative boundary layers. Micro shock tubes generally have a very low characteristics volume-to-surface ratio of less than 1:800. More over at low length scales and pressure values, the continuum assumption does no longer show accurate results as the molecular effects become important.

In micro scale flows Knudsen number (a non dimensional number) which relates the molecular free path to characteristic geometric length will be an important parameter. If the Knudsen number is less than 0.01, Navier Stokes equation based on continuum assumption will very well represent the flow physics and these modeling with the slip wall [8] assumptions can used up to Kn~0.1. When Knudsen number is more than 0.1 continuum approach is no longer valid and molecular dynamics studies should be used to represent the flow physics.

A detail study on the flow through micro tubes of various diameters has been carried out by Duff [1]. He found that the shock mach number reduces in a highly non linear manner with low initial driver section pressures. Later Brouillette [2] proposed a scaling factor, which relates the diameter and initial pressure to the shock attenuation. He proposed that less the former parameters more will be the shock attenuation. This has been further substantiated by Zeitoun [3] through his numerical studies on micro shock tube with various initial pressures. Ngomo [7] studied the effect of friction and heat losses for shock propagation in narrow tubes. Very few studies have been done till date to understand the shock propagation at low Reynolds number and low Knudsen number flows [4, 5, 6]. A more detailed study is required to identify the complete physics causing the shock attenuation and unsteady flow characteristics involved in micro scale shock tubes.

The objective of the present study is to numerically simulate unsteady flow evolution and shock propagation inside a micro shock tube. A micro shock tube of 5 mm diameter with H2/N2 as driver/driven gas has been considered for the present simulation and a complete rupture of diaphragm was assumed at the starting of analysis. A two dimensional model has been considered for the present study. The study aims at investigating the attenuation physics of shock propagation at various initial pressures, keeping the diaphragm pressure ratio
constant. The influence of slip wall boundary condition on shock propagation has also been investigated. A comparative study on the effect of slip and no slip wall boundary condition has also been made.

2. NUMERICAL SIMULATION

The computational domain consists of a driver and driven section with P4 higher than P1. The suffix 4 represents the driver section and 1 represents driven section.

Fig. 1 Shock tube geometry with 5 mm diameter

The domain was discretized into structured quad cells using ICEMCFD software. CFD analysis was performed in a commercial solver, Fluent. Numerical study was conducted for three cases which are listed below in Table 1. An axi symmetric model has been considered for the present study.

<table>
<thead>
<tr>
<th>Grid</th>
<th>Pressure Ratio</th>
<th>P1</th>
<th>Wall Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>25.04</td>
<td>100 Pa</td>
<td>No Slip</td>
</tr>
<tr>
<td>Case 2</td>
<td>25.04</td>
<td>10 Pa</td>
<td>Slip</td>
</tr>
<tr>
<td>Case 3</td>
<td>25.04</td>
<td>10 Pa</td>
<td>No Slip</td>
</tr>
</tbody>
</table>

Table 1: Initial conditions for different cases

A mesh independent study was carried out to eliminate the numerical errors associated with grid. The pressure value at different locations at a time of 0.1 μs has been monitored for all the three meshes and is shown in fig. 2. The third mesh which is not producing much deviation in results from its preceding mesh was used for all the future studies. Grid was densely clustered near to the wall to capture the boundary layer effects.

A compressible Navier Stokes equation was solved to predict the change in flow parameters. This equation has been coupled with the species transport equations to simulate the mass fraction variation of different species (H2/N2). Ideal gas equation has been used to predict the variation of density with respect to temperature and pressure. The material property variation of each species was modeled using ideal gas mixing laws. The flow has been considered as laminar and solved in an unsteady manner. Pressure based solver with simple algorithm for pressure velocity coupling has been used to solve the discretized equations. Temporal discretization has been done using second order implicit schemes and spatial discretization using third order MUSCL schemes. The driver and driven sections were patched with their corresponding initial pressures. All walls are assumed to be isothermal.

For the low initial pressure condition (Case-2) Knudsen number falls in the slip flow regime. At this condition flow will no longer attach to the wall but slips due to the molecular effects. The slip velocity and the temperature jump boundary condition have been mathematically modeled using the following equations.

\[ U_w - U_e = \frac{2 - \alpha_w}{\alpha_e} \frac{\partial}{\partial x} (U_e - U_c) \quad (1) \]

\[ T_s - T_w = \frac{2 - \alpha_g}{\alpha_e} \frac{\partial}{\partial x} (T_g - T_c) \quad (2) \]

Here the subscript g, w and e indicate gas, wall and cell-center velocities. \( \delta \) is the distance from the cell center to the wall. \( \alpha_w \) is the momentum accommodation coefficient of the gas mixture and \( \alpha_e \) is the thermal accommodation coefficient of gas mixtures. \( \lambda \) is the mean free path.

3. RESULTS AND DISCUSSION

The cases considered for the present investigation were having a theoretical shock mach number MS of 3 obtained from the ideal viscous shock tube equation. But numerical result shows a constant decrease of shock mach number with progress in time This is as expected due to the viscous losses produced by the boundary layer which is shown in fig 3. The velocity just downstream of the shock continuously degrades as it advances in length and this yields to deterioration in the momentum of the flow which is the leading factor for shock attenuation.
Figure 4 shows the shock wave propagation along the tube for Case-1, Case-2 and Case-3. All flow parameters have been plotted along the center line of the geometry. The shock position is obtained by identifying the location of the sudden jump in temperature and pressure values. It can be observed that the numerically predicted shock front always lag behind the ideal analytical solution. This attenuation effect will be more predominant when the diameter decreases or the initial pressure decreases as the core energy for the shock propagation will be destroyed by the viscous losses.

![Graph showing shock wave locations at different time D=5mm](image)

Fig. 4. Shock wave locations at different time (D=5mm)

The temperature plots for various time (Case-1) has been shown in figure 5. The temperature downstream of the shock is constantly decreasing as it advances and finally a stage will reach in which there is no energy for the shock to propagate and will get converted to compression waves.

![Graph showing temperature profiles at different time](image)

Fig. 5. Temperature profiles at different time

The starting of temperature jump represents the contact interface and the dip represents the shock location. The shock contact interface distance increases with progress in time which indicates that shock is moving faster than the contact surface. The same can be observed from the pressure plots versus time given in figure 6.

![Graph showing pressure profiles at different time](image)

Fig. 6: Pressure profiles at different time

The pressure, temperature and density distribution for Case-1 at a time of $2\times 10^3$ s has been shown in the figures 7, 8 and 9 respectively. Shock fronts have been numerically captured as a sudden jump in the above parameters. The shock wave moves into the driven section increasing the pressure. Similarly an expansion wave moves into the driver tube reducing the pressure. The shock-contact interface distance experience a rise in temperature and density as explained by the general moving shock equations.

![Graph showing pressure distribution at t=2x10^-4 s](image)

Fig. 7: Pressure distributions at $t=2\times 10^{-4}$ s

![Graph showing temperature distribution at t=2x10^-4 s](image)

Fig. 8: Temperature distributions at $t=2\times 10^{-4}$ s

![Graph showing density distribution at t= 2x10^-4 s](image)

Fig. 9: Density distributions at $t= 2\times 10^{-4}$ s

Figure 4 also shows the unsteady shock evolution for Case-2 (P1=10 Pa). Shock waves shows more attenuation
for this case and this shows that the shock position strongly depends on the initial pressure. When initial pressure is low the associated boundary layer growth will also be more. But the imposition of slip boundary on the walls reduces this effect. Slip will give additional velocity jump to the wall attached fluid layer and this will reduce the boundary layer effect. Figure 10, which shows the comparison of velocity distribution with and without slip, clearly explains this.

Fig. 10: Velocity distribution at t=2x10^{-4}s for Slip and No Slip conditions

A thicker boundary layer can be observed for low initial pressure no slip case (Fig.10-b) compared to the high initial pressure case (Fig.3). This shows that the boundary layer development has a strong dependency on the initial low pressure.

Figure 11 and 12 shows the temperature contour of case-2, at time 2x10^{-4} s, with and without slip wall respectively. It can be clearly noticed that slip wall reduces the losses and produce a more pronounced core flow.

Fig. 11: Temperature distributions with slip wall at t=2x10^{-4}s

Fig. 12: Temperature distribution without slip wall at t=2x10^{-4}s

The thermal boundary layer development for no slip case is more, which significantly reduces the core energy. The widely distributed temperature contour of no slip wall case shows that shock wave have almost transformed into a compression wave. Temperature at core is almost 355 k at 2x 10^{-4} sec where as for the case with slip effect considered is showing a temperature of 590 k. Because of the above reasons slip wall case shows more strong propagation of shock compared with no slip condition for same initial pressure and pressure ratio.

4. CONCLUSIONS

Computational studies were carried to investigate the unsteady flow evolution within a micro shock tube. The reasons for shock attenuation and its dependency on initial pressure conditions have been numerically studied. A strong attenuation of shock happens for low initial pressure situations. Slip wall conditions will become important at this low length scales as this will reduce the attenuation of shock movement. To numerically simulate more clear shock front warrants the inclusion of advanced flux discretization schemes and solution done in coupled manner. Also the influence of temperature on the material properties needs to be modeled. Further work is going on to incorporate these effects.

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