

CFD Analysis of Normal Shock using Shock Tube with Five Species

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Abstract: A shock tube is equipment that can produce a moving normal shock wave produced by the sudden bursting of diaphragm separating a high pressure gas section from one at lower pressure gas section. It is used in high speed test facilities. The objective is to solving shock tube problem with CFD code is to calculate the fluid flow property and observed how fluid parameters are varies with time because of shock tube used for high speed test and finding out the behavior of normal shock in the test field. In the present study, dimensional Euler equations are used as governing equation. The spatial discretization is carried out by unstructured cell-centered Finite Volume Method. Here the convective fluxes are evaluated using Van Leer Flux Splitting Scheme. Species transport equations are also added in the Euler equation for treatment of non-reacting mixing of the gas.

Keywords: Shock tube, Moving normal shock, Observation time in shock tubes, Euler equations, Finite Volume Method, Van Leer Flux Splitting schemes.

1. Introduction

Continuous effort is being made to increase the limit of maximum obtainable speed by mankind. Research and development towards this effort lead us to develop efficient and affordable test facilities. Day by day it is becoming difficult to ignore the short duration, high speed flow test facilities. This thing compelled us and increases our curiosity to know about the high speed flow test facilities. Interest has recently been revived by researchers towards this high speed flow conditions which can be used to simulate the real conditions encountered by aerospace vehicles in an apparatus which was first developed hundred years ago. Today, this apparatus is known as shock tube. Shock tube is developed to study about the high speed flow like supersonic and Hypersonic related to the aerodynamics of aerospace vehicles where some concepts such as heat transfer and high temperature effects are very important. Shock tube is developed to study such phenomena in laboratory condition which are not possible in actual flight conditions.

It is a device to produce high speed flow with high temperatures, by traversing normal shock waves which are generated by rupture of a diaphragm separating a high pressure gas from a low pressure gas. In the 19th century, interest in the propagation speeds of flame fronts and detonation waves led to the construction of the first shock tube by Pierre Vieille in France in 1899. Experimental work on shock tube has been carried out in the 1940s in the United States and Canada, where initial experiments were made to find a method of blast pressure measurement. It was later realized that shock tubes can be used to investigate compressible flow phenomena and extensive experiments on interactions of shocks, rarefactions and contact surfaces were made in Al-Falahi [1].

Various simulation software and solvers are being developed in the last decade to facilitate various aerodynamic analysis on supersonic and Hypersonic flow. Extensive analysis is carried out to study and design a one dimensional shock tube with configurations of single diaphragm shock tube. Effect of variation in pressure ratio, composition of driver gas is also studied in this report. All the analysis is being done using L1D (Linear One Dimensional) software. The problems are also solved analytically and solvers are also developed for the study.

2. Governing Equations

For high speed flows, viscous effect is confined to the vicinity of the surface, where the large velocity gradient exists. This region is known as the boundary layer. Outside of the boundary layer, the velocity gradients are negligible resulting in zero shear stress. This region is called the inviscid region. In the present study, the investigation of solution procedures for the inviscid flow region. The governing equation is known as the Euler equation [2]. In two-dimensional Cartesian coordinates, these can be written as

$$\frac{\partial \bar{U}_i}{\partial t} + \frac{\partial \bar{F}_i}{\partial x} + \frac{\partial \bar{G}_i}{\partial y} = 0 \quad (1)$$

$$\bar{U}_i = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \\ \rho m_i \end{bmatrix} \quad \bar{F}_i = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uH \\ \rho um_i \end{bmatrix} \quad \bar{G}_i = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vH \\ \rho vm_i \end{bmatrix}$$

The Euler equations governing the 2D flow in the absence of body forces with species transport equation in the conservative and differential form are,

$$\frac{\partial(\rho)}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} = 0 \quad (2)$$

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2 + p)}{\partial x} + \frac{\partial(\rho v u)}{\partial y} = 0 \quad (3)$$

$$\frac{\partial(\rho E)}{\partial t} + \frac{\partial(\rho u H)}{\partial x} + \frac{\partial(\rho v H)}{\partial y} = 0 \quad (4)$$

$$\frac{\partial(\rho m_i)}{\partial t} + \frac{\partial(\rho u m_i)}{\partial x} + \frac{\partial(\rho v m_i)}{\partial y} = 0 \quad (5)$$

In the above versions of formulations, the total specific energy, $E=e+0.5(u^2+v^2)$ the total specific enthalpy $H=h+0.5(u^2+v^2)$, is the mass fraction of the species given by $m_i=\rho_i/\rho$. This thesis considers a solution to unsteady state Euler equations and no surface forces are considered in these equations. Euler equation basically expresses the conservation of mass, momentum and energy.

2.1 Equations of State

The governing differential equations for the gas dynamics (i.e. Equation 2, Equation 3 and Equation 4) are completed by specifying the thermodynamic properties of the gas. For a perfect gas, the equation of state is

$$P = \rho RT \quad (6)$$

Where, R is the gas constant. And the speed of sound is given by $a = \sqrt{\gamma RT}$

The Thermodynamic properties of a number of ideal gases are given in the Table 1. For the mixtures of gases, the perfect gas relations can be used together with the effective thermodynamic properties or the mixtures of the gas, can be used the perfect gas relations together with the effective thermodynamic properties

$$R = \sum M_i R_i \quad \gamma = \sum M_i \gamma_i$$

Where, 'M_i' is % mass fraction of the species. Here, the summation is over the two species.

Table 1: Thermodynamic properties of ideal gases

| Gas | R (j / kgK) | γ |
|-----------------|---------------|------|
| Air | 287.0 | 1.4 |
| Helium | 2077.0 | 1.66 |
| Nitrogen | 296.8 | 1.4 |
| Argon | 208.0 | 1.66 |
| Co ₂ | 188.9 | 1.4 |

3. Numerical Method

3.1 Finite volume method formulation

The basic idea of a FVM is to satisfy the integral form of the conservation laws to some degree of approximation for each

of many adjacent control volumes which cover the domain of interest.

$$\frac{d}{dt} \int_{V(t)} \bar{U} dV + \oint_{S(t)} \bar{n} \cdot \bar{F} ds = 0 \quad (7)$$

The average value of U in a cell with volume V is

$$\bar{U} = \frac{1}{V} \iint U dV \quad (8)$$

Eq. 3.1 can be written as

$$V \frac{d\bar{U}}{dt} + \oint_{S(t)} \bar{n} \cdot \bar{F} ds = 0 \quad (9)$$

$$\frac{d\bar{U}}{dt} + \frac{1}{V} \oint_{S(t)} \bar{n} \cdot \bar{F} ds = 0 \quad (10)$$

\bar{U} is the average value of U over the entire control volume, \bar{F} is the flux vector and \bar{n} is the unit normal to the surface. And $\bar{F} = F_i \bar{i} + G_j \bar{j}$, is the total inviscid flux, upon integrating the inviscid flux over the faces of kth control volume the above equation becomes

$$\frac{\partial U_k}{\partial t} + \frac{1}{V_k} \left[\sum_{i=1}^{nf} \bar{F} \cdot \bar{n} ds \right]_k = 0 \quad (11)$$

Here, $\bar{n} = \frac{\Delta y_i}{\Delta s_i} \bar{i} - \frac{\Delta x_i}{\Delta s_i} \bar{j}$ and $\Delta s_i = \sqrt{(\Delta x_i)^2 + (\Delta y_i)^2}$

For the 2-D axi-symmetric problems the finite volume formulation is given by

$$\frac{d\bar{U}}{dt} + \frac{1}{V} \oint_{S(t)} \bar{n} \cdot \bar{F} ds = 0 \quad (12)$$

3.2 Upwind discretization

Upwind schemes use an adaptive or solution-sensitive finite difference stencil to numerically simulate the direction of propagation of information in a flow field. A general form of writing any upwind-type schemes are

$$u_i^{n+1} = u_i^n - \frac{a \Delta t}{\Delta x} [(u_i^n - u_{i-1}^n) + (u_{i+1}^n - u_i^n)] \quad (13)$$

The upwind scheme is stable if the following Courant Friedrich–Lewy condition (CFL) condition is satisfied. Here CFL condition is $|a \Delta t / \Delta x| \leq 1$. Scheme is the first order accurate explicit scheme with only one unknown u_i^{n+1} .

3.3 Van Leer flux splitting scheme

The Van Leer scheme tells general fluid flow contains wave speeds that are both positive and negative (so that eigenvalue information can pass both upstream and downstream), the basic idea behind all of these techniques is that the flux can be split into two components F^+ and F^- so that each may be properly discretized using relatively upwind stencils to maintain stability and accuracy [3].

If $M_{\perp} \geq 1$, then $F_{\perp}^{+} = F_{\perp}$, $F_{\perp}^{-} = 0$

If $M_{\perp} \leq -1$, then $F_{\perp}^{-} = F_{\perp}$, $F_{\perp}^{+} = 0$

If $-1 < M_{\perp} < 1$ then numerical normal flux
 $F_{\perp} = F_{\perp}^{+}(U_L) + F_{\perp}^{-}(U_R)$

$$F_{\perp} = \begin{bmatrix} \rho u_{\perp} \\ \rho u_{\perp} u + p n_x \\ \rho u_{\perp} v + p n_y \\ \rho u_{\perp} H \\ \rho u_{\perp} m_i \end{bmatrix}$$

$$\bar{F}_{\perp}^{\pm} = \pm \frac{\rho c (1 \pm M_{\perp})^2}{4} \begin{bmatrix} 1 \\ u \pm (-M_{\perp} \pm 2) \frac{c}{\gamma^{\pm}} n_x \\ v \pm (M_{\perp} \pm 2) \frac{c}{\gamma^{\pm}} n_y \\ \frac{q^2 - u_{\perp}^2}{2} + \frac{c^2}{2(\gamma^{\pm} + 1)} [(\gamma^{\pm} - 1) M_{\perp} \pm 2]^2 \\ m_i \end{bmatrix}$$

3.4 Boundary Conditions

Boundary conditions are specifications of properties or conditions on the surfaces of fluid domains and sub-domains, and are required to fully define the flow simulation. Boundary condition decides the solution of the governing equation.

For two dimensional inviscid flow problem the commonly encountered boundary conditions are, 2D solid boundary fluxes, Inviscid or slip wall boundary condition, Pressure extrapolation boundary condition, Mirror image boundary condition, Far field boundary condition.

4. Solver Validation

4.1 Flows through ramp in channel

The problem consists of a uniform flow being disturbed by a small disturbance, in this case the ramp. The supersonic flow through a ramp channel is a standard test case to study the oblique shock for validation of 2D inviscid flow solvers. Free stream condition in this case given by Table 1. To start with Euler computations, flow at inlet is supersonic, oblique shock will be generated at the wedge. Using the geometry the bottom wall is turned upward at the corner through a deflection angle, 15° that is, the corner of concave. The length of the channel is 1.2 meters and height is 1 meter. Structured mesh used to have a grid size of 200×200 . The grid consists of 80601 cells, 80000 points, 160600 faces. The flow geometry and corresponding computational mesh are shown in Figure 1.

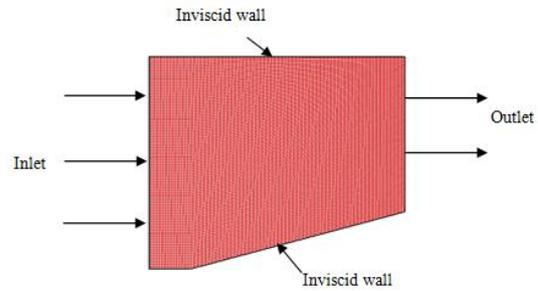


Figure 1: Grid for ramp in a channel

The lower wall, including the ramp, and the top wall are modeled as being impermeable boundaries i.e. Slip-wall boundary condition is imposed. For computation, first order scheme, with the Van Leer scheme is used for the calculation of the convective fluxes. The convergence criterion is based on the difference in density values, ρ , at any grid point between two successive iterations, that is,

$$|\rho^{n+1} - \rho^n| \leq 10^{-6}$$

Where, n is the iteration index.

The supersonic flow (Mach=3) at the wall must be tangent to the wall, hence the streamline at the corner also deflected through the angle 15° . Due to this free stream flow is “turned into itself” that is the oblique shock which is clear in present simulation. From the property of oblique shock theory the flow property must be increased. Figure 2 (a) shows the Mach number discontinuously decreases.

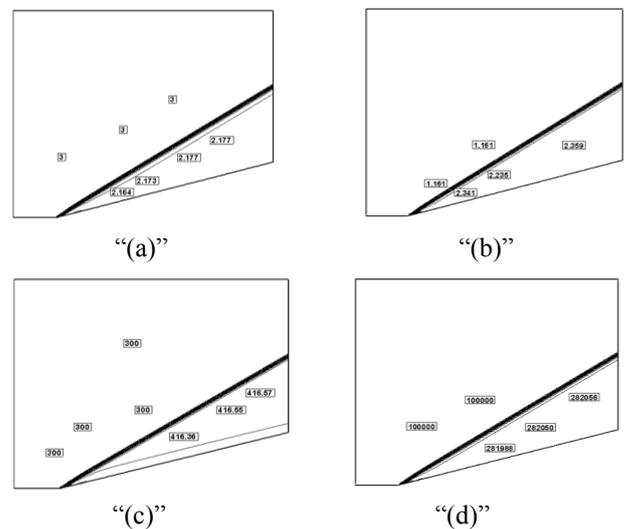


Figure 2: property contours in supersonic flow

The density, temperature and pressure discontinuously increases, which are demonstrated in Figure 2 (b), Figure 3 (c) and Figure 2 (d) respectively. In addition, for validation, the oblique shock properties computed from the present solver are in excellent agreement with the oblique shock relations [4] as shown in Table 3.

Table 2: Free stream condition for ramp in a channel

| Test case | Free stream input conditions | | | |
|-----------|------------------------------|------------------|------------------|-----------------|
| | M_∞ | U_∞ (m/s) | P_∞ in Pa | T_∞ in K |
| 1.66 | 3 | 1134.16 | 100000 | 300 |
| 1.105 | 3 | 1350.15 | 100000 | 300 |
| 1.4 | 3 | 1041.56 | 100000 | 300 |

Table 3: Comparison of various parameters across shock (wedge) for different species

| Parameter | Oblique shock theory | Solver Result with $\gamma=1.66$ |
|-----------------|----------------------|----------------------------------|
| P_2/P_1 | 3.143 | 3.005 |
| T_2/T_1 | 1.692 | 1.529 |
| ρ_2/ρ_1 | 1.992 | 1.994 |
| M_2 | 2.019 | 2.083 |
| B | 34.205 | 33.331 |

5. Result and Discussion

5.1 Shock tube problem 1D and 2D with various species

A shock tube consists of a long tube, usually of circular or rectangular cross section, which is separated by a thin diaphragm into two parts which is shown in Figure 3. One of them, the low pressure chamber, is a field with the test gas. The compressed driver gas fed into the second part, the high pressure chamber [5]. The dimension of the tube can vary.

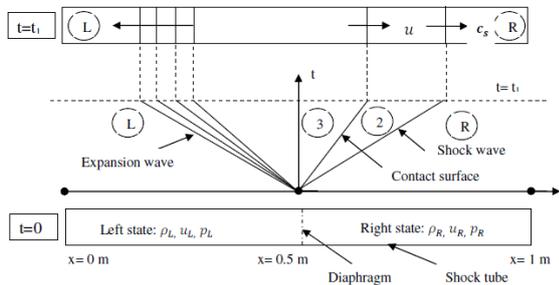


Figure 3: Schematic diagram of shock tube at time $t=0$, $t=t_1$

A shock tube is equipment that can produce a moving normal shock wave produced by the sudden bursting of diaphragm separating a high pressure gas section from one at lower pressure gas section. It is used in high speed test facilities. The objective is to solve shock tube problem by the solver to determine the fluid flow property under the tube.

5.2 Test condition of shock tube

The shock tube problem is the study of the propagation of shock waves in a one and two dimensional. Assume a neutral gas exists in the tube, as there are no charged particles. At the beginning, the system is divided into two parts with different pressure and density. The Initial condition for the solution is given by the Table 4.

Table 4: Initial condition for 1D, 2D and L1D shock tube

| Driver Section | | | | Driven Section | | | |
|----------------|-----------------|-----------------|---------------|----------------|-----------------|-----------------|---------------|
| Gas | u_L in m/s | p_L in bar | t_L in K | Gas | u_R in m/s | p_R in bar | t_R in K |
| Helium | 0.0 | 2.5 | 300 | Air | 0.0 | 0.1 | 300 |

The first, 1D case, divide the one dimensional space of the present simulation into 1000 uniform grid points as shown in Figure 4. The total length of the simulation region is 1 meter, so the ($\Delta x=0.01$).

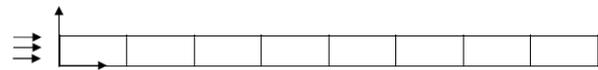


Figure 4: Schematic of 1D grid for shock tube (Not to scale)

Second, for the 2D case, the geometry of the shock tube used is as follows: The length of the tube is 1 meter and height is 0.4 meters. The grid consists of 6191 cells, 6000 points, 12190 faces. The flow geometry and corresponding computational mesh are shown in Figure 5.

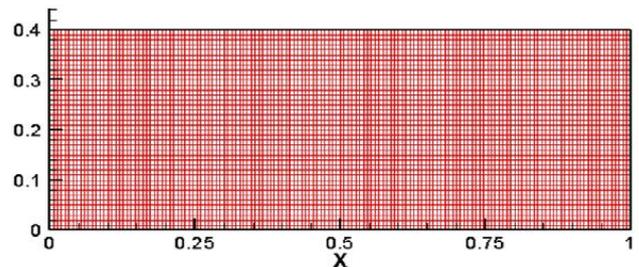


Figure 5: Schematic of 2D grid of shock tube

Here two cases are solved by the solver. For computation, first order scheme is used for discretization, which means that only one step is needed to finish a round of computation. For time, a uniform time step is adopted for simplicity that is, $t=0.004$. It cannot be sure that this is right, after check the result to see whether the time step is sufficient. If not, change the step.

The stability criterion is based on time for both the cases, that is,

$$\Delta t \leq \Delta t_{allowed} = CFL \times \Delta t_{signal} \quad (14)$$

where, $\Delta t_{allowed}$ smallest value for all cells and CFL is the specified Courant- Friedrich- Lewy number. It is normally restricted to $CFL \leq 1.0$. Here the CFL number is set to 0.3. For each cell, the invicid signal time for 1D and 2D case is approximated as Equation 7 and Equation 8 respectively.

$$\Delta t_{signal} = \frac{\Delta x}{|u_j| + c_j} \quad (15)$$

$$\Delta t_{signal} = \left\{ \frac{\Delta x}{|u_{i,j}| + c_{i,j}} + \frac{\Delta y}{|u_{i,j}| + c_{i,j}} \right\} \quad (16)$$

From the Figure 6, Figure 7 and Figure 8 shows the result of shock tube problem (1D and 2D) at time $t=0.4$ ms, together with the analytical solution (L1d, which gives exact result for shock tube) result of the problem at the same time [6]. The simulation result fits the basic configuration of analytical result quite well. We can also see clearly that diffusive error is very obvious in some part of the result and all the corners are smoothed. These plots are generated only after the bursting of diaphragm.

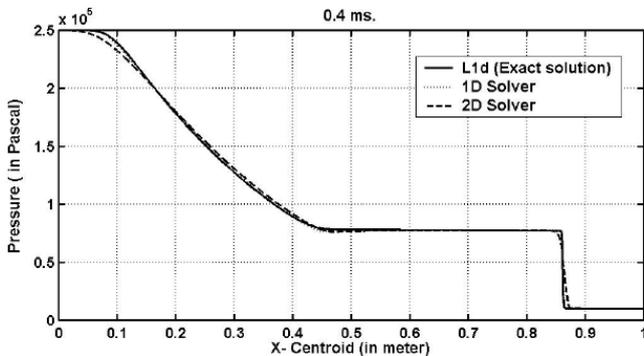


Figure 6: Pressure variation along a simple shock tube

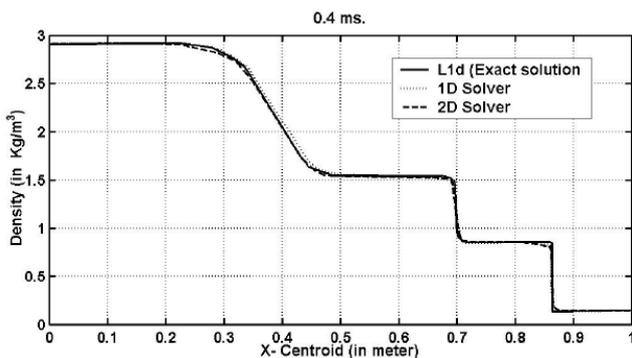


Figure 7: Density variation along simple shock tube

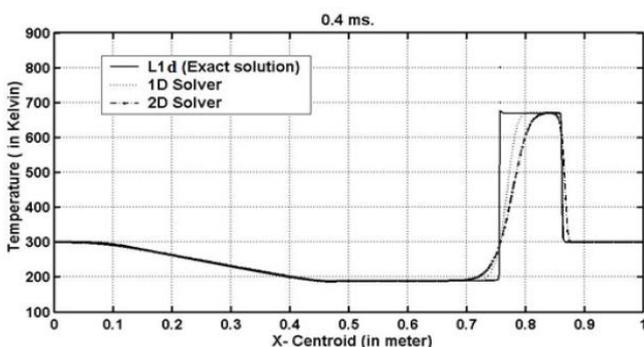


Figure 8: Temperature variation along simple shock tube. Also assume that there is no motion at the beginning. Figure 9 shows the state of the shock tube at $t=0$. From the contour representation of 2D shock tube case shows the effects of the moving shock wave propagation which is clear in Figure 10, Figure 11 and Figure 12.

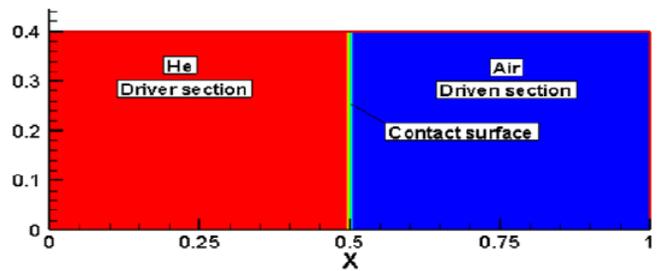


Figure 9: Diaphragm position at $t=0$ before bursting

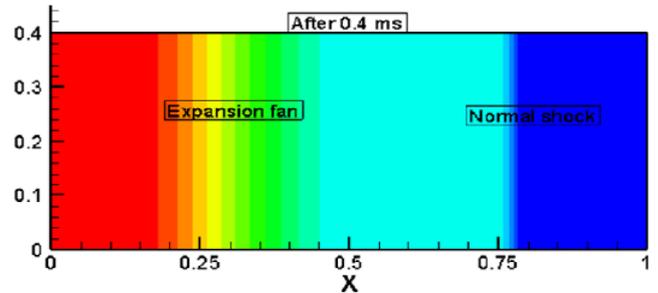


Figure 10: Pressure contour at $t=0.4$ ms in shock tube

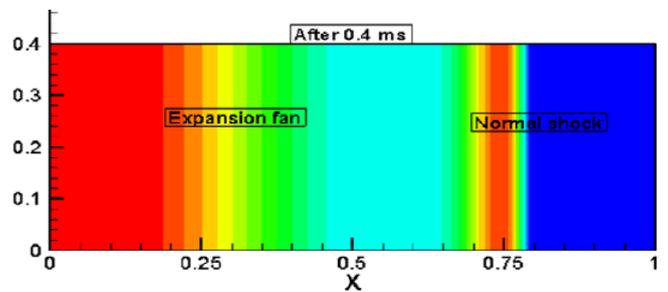


Figure 11: Density contour at $t=0.4$ ms in shock tube after diaphragm

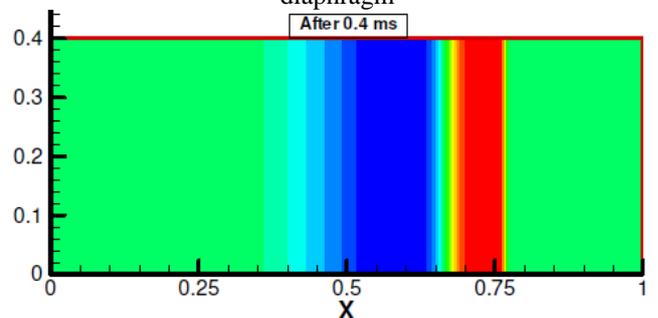


Figure 12: Temperature contour at $t=0.4$ ms in shock tube after diaphragm

6. Conclusion

The work has been carried out keeping in mind that this project is about numerical simulation through different solver and thus design of a one dimensional shock tube with configurations of single diaphragm shock tube is done. The simulation has been done to reach the supersonic Mach number 3.0 and the solver facilitates measurement of the properties behind the normal shock wave and their variation across the shock. Simulation is done using different pressure ratio across the shock in order to get wide range of Mach number. From results of CFD simulation for reflected wave shock tube, one can conclude that Van leer Flux Vector Splitting Scheme cannot be applied for low Mach number

flows but can be successfully applied for the supersonic and hypersonic flows. A good match has been found between CFD results and the L1D results.

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