Performance evaluation of shock tube with helium and carbon dioxide using numerical simulation

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Abstract. This work deals with the performance of the shock tube with helium and carbon dioxide as working fluids at different diaphragm pressure ratios using numerical simulation. A two-dimensional planar geometry of the shock tube is considered for the study. An inviscid time accurate model is developed to find the effects of diaphragm pressure ratios on the shock Mach number, temperature behind the incident and reflected shocks. This numerical model is validated analytically as well as experimentally with air as working gas. Simulations were conducted for same and different driver/driven gas combinations with helium and carbon dioxide test gases using this model. Simulations were carried out using CFD solver FLUENT. Adaptive Mesh Refinement (AMR) technique was applied to accurately capture and resolve shock and contact discontinuities. At lower pressure ratios the different gas model is able to produce 20.4% and at higher diaphragm pressure ratios up to 33% increase in shock Mach number when compared to the similar driver-driven gas model.

1. Introduction
The shock tube is an experimental test facility in which a plane propagating shock is created for short time intervals is produced in a long duct by the abrupt rupturing of the diaphragm separating a high pressure and low-pressure regions. Shock tube in its simplest form consists of a uniform area duct with both ends closed, which is divided into the driver and driven sections by a diaphragm. Initially these sections filled with a high-pressure gas in the driver and low-pressure gas in driven sections respectively. When the pressure difference is enough to break the diaphragm, the driver gas will push through the driven gas like a piston resulting in a shock wave. The incident shock wave moves in the lower pressure side by heating and compressing the driven gases. At the same time, an expansion or rarefaction wave moves back into the driver side. Both waves reflect off by the end walls. The shock tube is a versatile experimental facility for the study of chemical kinetic behaviour of gases at elevated temperature and pressure. By analysing the different combination of driver and driven gases, it is possible to identify suitable gas combination for various purposes.

Ideal shock tube flow is shown in figure 1. The right side of the diaphragm is of low pressure which is the experimental gas subjected to the shockwave. The high-pressure side, containing driver gas (state 4), is shown in left side of the diaphragm. The diaphragm is assumed to be ruptured right away at time t=0. After the rupture compression waves are formed in the driven side. The region behind this rapidly steepening to form a shock front is state-2. An abrupt rise in temperature and pressure is observed in this region. Simultaneously, an expansion or rarefaction wave moves back into the driver side. But the pressure drop is smooth and gradual. This rarefaction wave is often referred to as “expansion fan”. And
the region behind expansion fan is state-3 having lower pressure and temperature. The contact surface is referred to as the region formed by experimental gas and the driver gas, which moves rapidly along the direction of the shock front. End walls reflect shockwave as well as expansion fan. Reflection causes additional heating and compression and this region is state-5. And state-6 is the region behind reflected expansion wave.

Figure 1. Ideal shock tube flow

Most of the earlier studies modelled shock tube flow as one dimensional, which fails to simulate nonlinear physical processes, whereas multidimensional simulations can accurately model the unsteady flow. B. M. Argrow [1] simulated the growth of the wave field of a van der Waals gas with the use of a TVD predictor-corrector scheme with a reflective end wall boundary condition. Mouna Lamnaouer [2] conducted extensive numerical simulations over a shock tube with a variable area of cross-section. Ananthu JP [3] numerically modelled the flow inside shock tube and validated theoretically using the Rankine Hugoniot normal shock relation. K.P.J Reddy [4] had discussed about simple hand operated shock tube capable of producing Mach 2 shock wave. M. A. H Mohammed [5] explains a scheme that utilizes the AUSM flux splitting method for shock capturing. Al-Falahi Amir [6] developed a new two dimensional accurate Euler solver which uses 2nd order accurate finite volume special discretization and 4th order accurate Range-Kutta temporal integration used for the parametric study of hypersonic test facility. Yigang Luan [7] investigated the flow field inside a shock tube with a small nozzle at the end plane with second-order ROE numerical schemes.

The above studies gave an insight into the various non-ideal phenomenon and flow evolution in shock tube that affects the test time. Multi-dimensional models give better accuracy in modelling unsteady and highly non-linear processes when compared to simple 1-D models.

The aim of this study is to accurately predict the advantages of using different gas model over the same gases at the driver and driven sections. By analysing the different combination of driver and driven gases, it is possible to identify suitable gas combinations for various purposes. Time accurate two-dimensional model has been developed to conduct the parametric study. Propagation and reflection of shockwaves are investigated using this model. Viscous effects are neglected to reduce calculation times and for inviscid flow, Navier Stokes equations get reduced into Euler form. For better resolution of shock and contact discontinuities, adaptive mesh refinement method was applied to time-dependent flows. Model is made with ICEM CFD and numerical simulations were carried out in CFD solver Ansys FLUENT 18. Validation of the inviscid model is made by comparing with the analytical solution as well as experimental results. This model is used to simulate helium-helium, helium-carbon dioxide and carbon dioxide-carbon dioxide test gas combinations in the driver and driven sections respectively.
2. Numerical Modelling

2.1. Governing Equations

The flow is assumed to be inviscid for modelling of highly non-uniform conditions caused by intricate mechanisms responsible for reduced test times in the shock tube. Euler equation is basically a quasi-linear hyperbolic partial differential equation. The conservative form of the Euler equation in Cartesian coordinate two dimensions is given by:

\[
\frac{\partial U}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} = 0
\]  

(1)

Where vectors \( U, E \) and \( F \) are given as:

\[
U = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \epsilon \end{bmatrix}; E = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ u(\epsilon + p) \end{bmatrix}; F = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ v(\epsilon + p) \end{bmatrix}
\]  

(2)

Specific Energy is given by:

\[
\epsilon = \frac{1}{\gamma - 1} \left( p - \frac{1}{2}(u^2 + v^2) \right)
\]  

(3)

Pressure:

\[
p = (\gamma - 1) \left( \epsilon - \frac{1}{2} \rho (u^2 + v^2) \right)
\]  

(4)

Where \( U \) represents the conserved variables \( E \) and \( F \) are the overall fluxes in \( x \)-, \( y \)-directions respectively. And \( \rho, u \) and \( v \) represent the density and velocity per unit mass of the fluid in \( x \) and \( y \)-direction respectively.

2.2. Flow Domain

Shock tube domain consists of an inner diameter of 29cm and 650cm length. A two-dimensional approach to the cylindrical geometry of the shock tube gives a rectangular flow domain adequate to render precise information of the real flow configuration. It is divided into driver section of 50cm and driven section of 600cm by length as represented by figure 2. The complete domain of the shock tube is modelled. Since, we require the entire flow domain has to be simulated. Computations are carried out with helium-helium, carbon dioxide-carbon dioxide and helium-carbon dioxide gas combinations in the driver and driven sections.

Figure 2. Schematic Diagram of computational domain

2.3. Meshing

The meshing of the flow domain is done by the uniform quadrilateral method. The domain is divided into 20000 nodes. In the structured mesh grid lines are aligned to the direction of flow. So accurate solutions can be obtained. Initially, a base coarse grid is used and as the solution proceeds, to increase the computational efficiency Adaptive Mesh Refinement technic is used for regions with the steepest density gradient. AMR technique was effectively used to create a cluster of cells around the density gradient region as shown in figure 3. Added finer sub-grids to the regions of steepest density gradients gives better simulation results. Dynamic adaptation maintains the finer mesh around the shock and
increases the accuracy of the solution. This technique will reduce the overall computational time without sacrificing accuracy. The figure shows the mesh before starting iterations. At t=0 the contact discontinuities will be at the diaphragm region which will add additional nodes at the same location. When solution proceeds additional cells are added around both incident shock and expansion fan.

![Figure 3. Initial grid around diaphragm section](image)

2.4. Initial and boundary conditions
The shock has closed ends at left and right boundaries of the computational domain. So solid wall boundary is assumed. The mass flow in the momentum equation won’t penetrate through the solid wall ends. Initial flow variables at each point of the flow domain are specified before performing the iterations. The initial solution of the problem consists of two uniform states separated by a discontinuity at 50cm from the left end. Pressure values are given at both driver and driven sections according to the desired pressure ratio. The temperature of driven and driver regions are taken as 302K. The pressure at the driver section (P4) is fixed to 6atm and driven section (P1) is varied from 1atm to 0.2atm to get diaphragm pressure ratios 6 to 30. Initially, the fluid is in stagnation condition and the simulations are carried out for different initial conditions.

| $P_1$ (atm) | Helium-helium | Carbon dioxide-carbon dioxide | Helium-carbon dioxide |
|-------------|----------------|-------------------------------|----------------------|
|             | $\rho_4$ (kg/m$^3$) | $P_1$ (kg/m$^3$) | $\rho_4$ (kg/m$^3$) | $P_1$ (kg/m$^3$) |
| 1           | 0.969           | 0.161                         | 10.653               | 1.775               |
| 0.8         | 0.969           | 0.129                         | 10.653               | 1.420               |
| 0.6         | 0.969           | 0.097                         | 10.653               | 1.065               |
| 0.4         | 0.969           | 0.065                         | 10.653               | 0.710               |
| 0.3         | 0.969           | 0.048                         | 10.653               | 0.532               |
| 0.2         | 0.969           | 0.032                         | 10.653               | 0.355               |

2.5. Numerical Scheme
The discretized model equations in space and time are solved with the control volume approach and density-based explicit solver. The choice of the solver is made based on the travelling shock and time-dependent solution. Flux vectors are computed with Advection Upstream Splitting Method (AUSM). In AUSM inviscid flux at cell interface is split into pressure and convective contributions. Pressure is upwinded based on acoustic considerations and convective is second order upwinded in the direction of flow. An explicit time stepping integration is performed using four stage Runge-Kutta scheme for unsteady flow. Time step is restricted to the stability limit set by the Courant-Friedrich-Lewy (CFL) condition.

3. Validation
The validation of the developed numerical model is done with the comparison of flow properties obtained from the simulation to the one-dimensional analytical solution of ideal theory relations and experimental values. The ideal theory solution is based on the solution of multiple gas dynamics relations called the Rankine-Hugoniot relations. Numerical simulations were conducted by taking air in
both the driver and driven sections for various pressure ratios to get the shock Mach number which sets the properties of the flow behind the incident shock and reflected shock. Experimental data was collected from the hand-driven shock tube for various pressure ratios obtained by evacuating the driven tube to various levels. The general trend shows that the inviscid model and ideal shock theory are in good relation. In the experimental data, the loss in shock Mach number for a particular diaphragm pressure ratio is a result of viscous losses and real diaphragm rupture times. Figure 4 shows the diaphragm pressure ratio’s corresponding to the shock Mach numbers. Figure 5 shows the temperature behind the reflected shock to the shock Mach numbers. Both values from the 2-dimensional inviscid model and the 1D ideal theory are compared. The results show that they are in perfect agreement as expected. This validated model is used for performing simulations with the different driver and driven gases.

**Figure 4.** Diaphragm pressure ratios vs incident shock Mach numbers (Ms).

**Figure 5.** Temperature behind the reflected shock vs incident shock Mach numbers (Ms).

### 4. Results

Simulations are conducted for various diaphragm pressure ratios ranging from 6 to 30. The results obtained by using the air as the working fluid is validated analytically as well as experimentally. Three models are considered to analyze the difference between using the same gas and different gas on the driver and driven sections. The first and second model consists of similar gases working medium in both driver-driven regions. So helium in first and carbon dioxide in the second model is used as a working medium. In the third model, helium is taken in the driver section and carbon dioxide in the driven section. Parametric analysis is conducted by comparing the properties of the flow behind the incident and reflected shocks in all cases. Effect of diaphragm pressure ratio on the temperature values at the heals of the incident shock and reflected shock are also studied.

**Figure 6.** Contours of pressure (in pa) (a) Initial condition (b) After the rupture of diaphragm.
Figure 7. Contours of temperature (in K) (a) After diaphragm rupture (b) Shock wave reflection from end wall creating high temperature region.

Figure 6 (a) shows the pressure distribution for an initial diaphragm pressure ratio of 6 with helium as driver gas and carbon dioxide as the driven gas. Pressure contours resolving incident shock and expansion fan are shown in Figure 6 (b). The temperature contour differentiates all the three discontinuities including contact surface as shown in Figure 7.

The comparison of diaphragm pressure ratio required for generating shock Mach number for the same gas and different gas models is shown in figure 8. As the diaphragm pressure ratio increases shock Mach number also increases as expected for all models. At lower pressure ratios helium-argon model shows 20.4% hike in Mach number compared to argon-argon. And at higher pressure ratios it’ll increases up to 33%.

Figure 8. Diaphragm pressure ratios vs shock Mach numbers (Ms)

Figure 9 compares the effect of diaphragm pressure ratio on temperature behind the incident shock wave. The helium-helium gas model gives the highest temperature T2. The different gas model shows intermediate temperature behind the incident shock. A total rise of 128K is observed for the different gas model. Total hike in temperature behind incident shock wave for helium gas model when compared to different gas model is found to be 30K at higher diaphragm pressure ratios.

Figure 9. Dependency of diaphragm pressure ratio on ratio of temperature of shocked gas to initial temperature.

Figure 10. Dependency of diaphragm pressure ratio on ratio of temperature behind reflected gas region to initial temperature.
Figure 10 shows the diaphragm pressure ratio required for generating temperature behind the reflected shock. As the pressure ratio across diaphragm increases the temperature behind the reflected shock also rises for both models as expected. However, the temperature behind helium-carbon dioxide model is less compared to carbon dioxide same gas model. As diaphragm pressure ratio increases from 6 to 30, increase in temperature behind the reflected shock is 243K for the helium-carbon dioxide model and 315K and 160K for helium and carbon dioxide same gas models respectively. The temperature T5 for a different gas model is 116K to 188K less than that of the same gas model as the pressure ratio changes from 6 to 30.

5. Conclusion

Two-dimensional shock tube geometry is simulated using the inviscid model with varying time step taking helium-carbon dioxide, helium-helium and carbon dioxide - carbon dioxide combinations in the driven and driven sections. Parametric studies on different diaphragm pressure ratios were conducted and the effect on incident shock Mach number, temperature behind the incident and reflected shocks were compared for both models. 20.4% hike in shock Mach number is observed at lower pressure ratios which increases up to 33% at higher pressure ratios. There is no significant advantages in temperature behind the incident and reflected shocks are observed for different gas model compared to the same gas model.

6. References

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