Numerical Investigation of the Impact of Tailored Driver Gases and Driver Inserts on Shock Tube Flows

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1 Introduction

The shock tube as a chemical reactor is used to investigate fundamental chemical kinetics such as rate constant measurements, ignition and pyrolysis processes. Resulting experimental data sets play a central role in the development of validated kinetic models for combustion analysis. The reactor is particularly attractive because of its ability to instantaneously generate conditions of high temperature and pressure. Ideally, the post-reflected shock region closely approximates a constant volume reactor, with the pressure and temperature remaining fairly constant until interaction with the reflected expansion wave or onset pronounced heat release as in ignition processes. The post-reflected shock pressure, commonly designated P_5, is readily measured in the shock tube and from pressure measurements one can approximate the Mach number of the shock front. Due to the short observation time windows, post-reflected shock temperatures are generally deduced from 1D shock relations using initial reactor conditions and the incident shock velocity as input variables.

Non-ideal behaviors in real shock tubes affect thermodynamic conditions of the post-reflected shock region and the time over which constant p_5 and T_5 can be observed may be severely limited. In low temperature experiments long times are need to measure ignition delays and the available time is effected by the properties of the driver gas. The method of contact surface tailoring through modified driver gas composition can be used to extend the test time

Further, non-ideal pressure rise that occurs in the post-reflected shock region can be controlled by reflecting weak expansion waves from the initial expansion fans by using shock tube driver inserts. The effect of the non-idealities on the conditions in the post-reflected shock region, most importantly T_5, are of interest and can only be reasonably quantified by, at least, 2D numerical studies.

The importance of shock tube data in the development and validation of chemical kinetic mechanisms calls for special attention in the generation and interpretation of shock tube data [1, 2]. Shock tube non-ideal behaviors such as the diaphragm rupture, the interaction of the reflected shock wave and the boundary layer, and the interaction of the reflected shock and contact surface can all contribute to changes in the test section and the difficulty in interpreting measurements made in the shock tube, and discrepancies between experiments and models. Shock tube driver gas tailoring and driver inserts can be used to reduce the impact of non-ideal behaviors on the post-reflected shock region and make interpretation of experiments easier. Driver gas tailoring has been studied extensively, and the conventional method is explained in Gaydon and Hurle [3], Glass and Sislan [4], and Nishida [5]. Experimental studies of contact surface tailoring have been conducted, such as those of Brabbs and Belles [6]. Unconventional driver gas mixtures were studied experimentally by Amadio et al. [7] and a theoretical model for driver gas mixtures in shock tubes with area change in the diaphragm section was developed and tested by Hong et al. [8]. Computational shock tube studies by Lamnaouer [9] included numerical investigations of different mixtures to identify one that yielded the longest test time for long ignition delay measurements in shock tubes. Driver inserts have been implemented to maintain constant pressure conditions in the post-reflected shock region. A design methodology was discussed in Hong et al. [10] and are used in Campbell et al. [11]. This paper is part of a number of numerical investigations aimed at better understanding shock tube flows and the impact of variations of established conditions on combustion chemical kinetics. The focus of this work is on the effects of imperfect tailoring and the use of driver inserts on the thermodynamic conditions in the test section. The flow field changes due to the coupling of driver gas tailoring and the driver insert and the chemical kinetic implications.

2 Simulation Methodology

Numerical simualtions of the gas dynamic flow in a cylinderical shock tube are carried out. The Navier-Stokes equations in integral form are solved and can be written in the form

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial}{\partial x_j}(\mathbf{F_j^c} - \mathbf{F_j^v}) = \mathbf{S} \tag{1}$$

$$\mathbf{U} = (\rho, \rho u_i, \rho e, \rho Y_n)^T; \tag{2}$$

$$\mathbf{F_j^c} = (\rho u_i, \rho u_j u_i + p\delta_{ij}, u_j(\rho e + p), \rho Y_n u_j)^T \tag{3}$$

$$\mathbf{F_j^v} = (0, \tau_{ij}, u_i \tau_{ij} + q_{ij}, \rho Y_n V_{jn})^T; \tag{4}$$

where $\mathbf{U}$ is the state vector, S is the source term, $\mathbf{F_j^c}$ and $\mathbf{F_j^v}$ are convective and diffusive fluxes, respectively. The gas species in the simulation are assumed to be non-reactive, and are treated using the ideal gas model. To model temperature effects on the transport properties, the dynamic viscosity of each gas component is modeled with Sutherland's Law, and the thermal conductivity calculated using the modified Euken model. Specific heat dependence on temperature was modeled using JANAF polynomials. Further the cylindrical shock tube is modeled as axisymmetric, providing a 2D simulation to take into account the effects of walls on the shock wave structure. For the energy equation the walls have been treated as adiabatic walls. The driven gas is Argon, chosen for its wide use in high proportion as a diluent in shock tube studies. For the driver gas mixture, Helium and Nitrogen are used.

Table 1: Average Pressure and Temperatures in post-reflected shock region before disturbances.

Condition He/N_2	Δt [ms]	P5 [atm]	T5 [K]
Tailored	6.72	2.88	1544
50-50 Over	2.81	2.90	1556
75-25 Over (weak)	2.83	2.90	1554
90-10 Under	2.23	2.87	1543

The shock tube simulated has a driven section of 4.0m and a driver section of 2.7m. The entire length of the shock tube is simulated, taking advantage of the axisymmetric assumption half of the shock tube is simulated. The domain is decomposed with 4000 cells along the axis of the shock tube and 40 cells along the radial direction. In addition to capture near wall behavior the grid was stretched along the raidal direction, with smaller cells close to the wall, with a minimum radial cell spacing of 0.11544mm and a cell-to-cell expansion ratio of 1.1.

The Navier-Stokes equations are solved using the density-based solver rhoCentralFoam of the open-source software OpenFOAM. The rhoCentralFoam code uses a semi-implicit scheme based on the central schemes of Kurganov and Tadmor [12]. Time integration is explicit using a forward Euler method and spatial operators are discretized with second order accurate discretization. The van Albada limiter is used to capture the shock fronts and the contact discontinuity. For stability of the simulation the time step size was adjusted to maintain a CFL number of 0.125.

3 Results and Discussion

Table 1 gives the driver gas mixtures in mole percentage used in this set of simulations. The mixtures represent the possible tailoring conditions that can occur under, over and perfectly tailored, In addition the test section pressure and temperatures calculated from simulations are given. Initial conditions in the bottom three cases are made to obtain approximately similar post-reflected shock conditions. Figure 1 shows the temperature field in the driven section of the shock tube after the reflection of the incident shock wave.

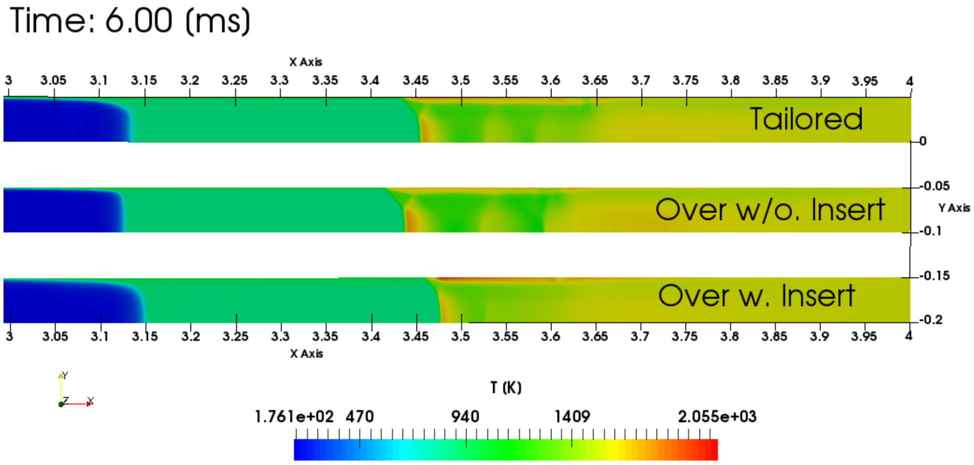

Figure 1: Temperature field in the driver section of shock tube. Reflected shock wave is traveling towards contact surface

Three cases are displayed for comparison, the first contour shows the temperature field produced when a tailored driver mixture is used to drive the shock wave. The next two cases use the same over-tailored driver gas mixture, one with a driver insert and the other without. Figure 2 shows the temperature field of the same cases at a later time. The reflected shock wave and contact surface have interacted. The interaction between the contact surface and the reflected shock wave has led to an instability, resulting in a mixing zone rather than well defined interface. In the case of the over-tailored driver mixture this mixing zone continues to move towards the test section at the end wall. Compressive waves are developed that travel to the end wall and lead to increases in temperature and pressure in the measurement section that will have implications on chemical kinetics measurements.

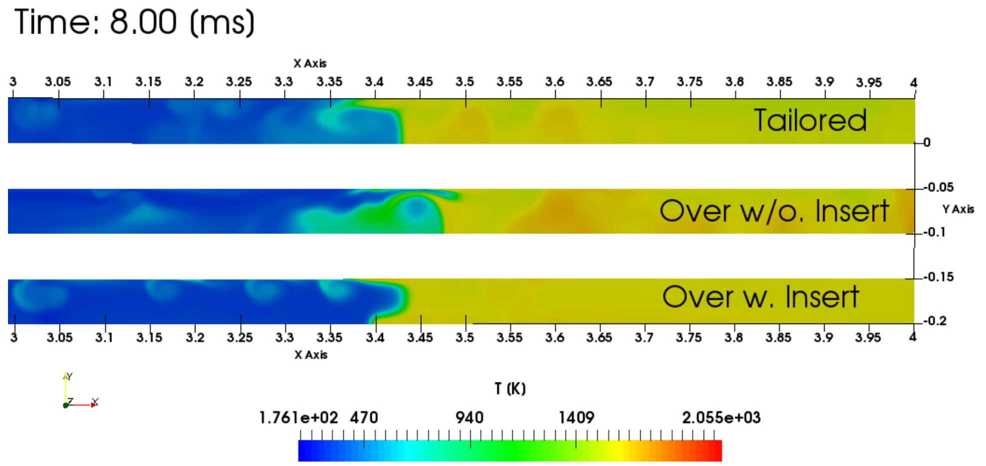

Figure 2: Temperature field in driver section of shock tube. The contact surface after interaction with reflected shock wave

For accurate chemical kinetic measurements it is important to have nearly uniform temperature and pressure in the measurement section of the shock tube until the chemical reaction has taken place. Figure 3 shows computed pressure time histories probed at a location near 1 cm from the end wall of the shock tube. In this figure the tailored driver mixture and an under-tailored driver mixture are compared to illustrate the increase in testing time that is to be expected from tailoring of the driver gas. Oscillations in the pressure histories are due to wave processes generated by the interaction between the reflected shock wave and the contact surface.

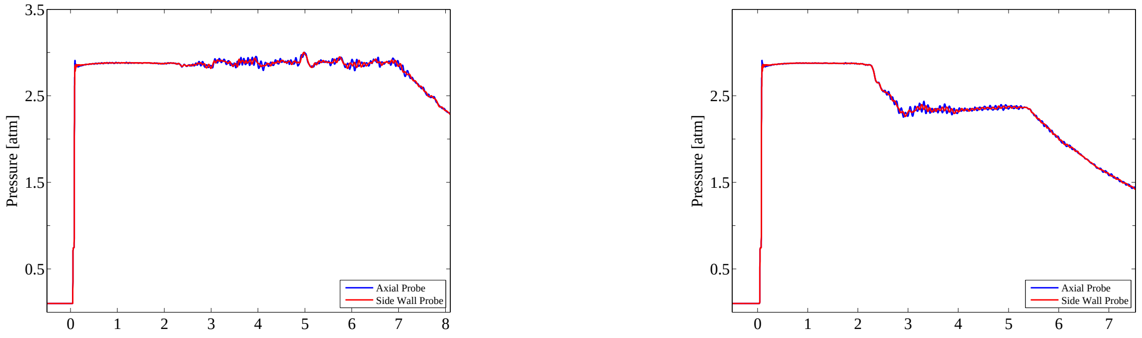

Figure 3: Pressure and Temperature profile in post-reflect shock region, 1cm from end wall for tailored and under-tailored driver mixtures.

In figure 4 we compare the effects of the driver inserts on the control of pressure and temperature increases. The over-tailored driver gas case is used and an insert contour was designed to manage the pressure rise due to the compression waves generated by the over-tailored contact surface. The first important observation is the sudden temperature decrease in the case without the driver insert, due to the Richtmyer-Meshkov instability that was seen to develop in figure 2 low temperature driver gas was forced to the end wall. This behavior is absent in the case with the driver insert, as the weak expansion waves not only weakened the compression waves but the instability at the contact surface. Another interesting observation is that the combination of the over-tailored driver mixture and the driver insert has extended the time of arrival of the expansion fan, and lead to a test time approximately 1 ms longer than that of the tailored gas case.

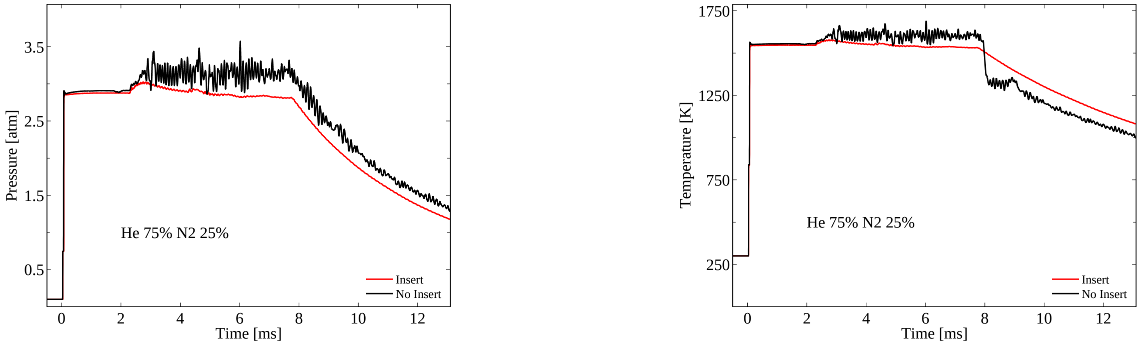

Figure 4: Pressure and Temperature profile in post-reflected shock region, located at 1cm from end wall. Comparison between mild over-tailored case with driver insert and without driver insert

The effect of changes in the thermodynamics state of the test gas as a result of imperfect tailoring is assessed by applying proportionate changes in temperature and pressure during ignition of a stoichiometric mixture of 1% iso-propanol in oxygen and argon mixtures at about 2.21 atm. The results are shown in Fig. 5, where the test time extension because of the cooling brought about by the under-tailored behavior stands out prominently. This assessment points to the need to carefully analyze effects of tailoring on the resulting thermodynamic conditions and their implications on kinetic time scales.

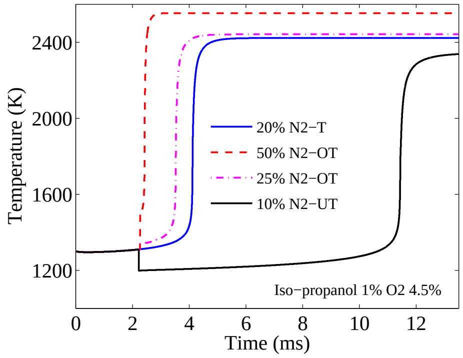

Figure 5: Effect of pressure and temperature changes due to imperfect tailoring on the ignition delay time simulation of a stoichiometric mixture of 1% iso-propanol in oxygen and argon at 2.21 atm 1300 K post-reflected shock conditions.

4 Conclusion

In this work we completed numerical simulations of a shock tube geometry with several driver gas mixtures representing the different conditions possible in driver gas tailoring. A second shock tube geometry representing a shock tube with driver section insert was completed for a weakly over tailored driver gas case. The contour of the insert was designed to reduce the effect of the compression wave due to the deviation of the driver gas mixture from that of a perfectly tailored mixture. The main goal of these experimental techniques is improve the testing time available in the shock, and to obtain near uniform pressure and temperature conditions in the test section. As expected, the driver gas tailoring technique can extend the measurement time significantly, but obtaining perfectly tailored gas mixtures is challenging. The combination of the weakly over-tailored driver mixture and the driver insert lead to a test time approximately 1 ms longer than the tailored driver mixture case. In addition, the weak expansion waves had an effect on the contact surface instability observed in the over-tailored case.

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