Optimization of Pressure and Temperature Characteristics of a High

Pressure Shock Tube

ΒY

JAI M. MEHTA

Diploma in Mechanical Engineering, S.B.M. Polytechnic, Mumbai-India , 2013 B.E. , University of Mumbai , Mumbai-India, 2016

THESIS

Submitted as partial fulfillment of the requirements for the degree of Master of Science in Mechanical Engineering in the Graduate College of the University of Illinois at Chicago, 2018

Chicago, Illinois

Defense Committee:

Kenneth Brezinsky, Chair and Advisor, Mechanical and Industrial Engineering Robert S. Tranter, Argonne National Laboratory Patrick T. Lynch, Mechanical and Industrial Engineering This thesis is dedicated to my parents, Sonia M. Mehta and Manoj K. Mehta, without their unconditional love and support

this would not have been accomplished.

ACKNOWLEDGEMENTS

I am grateful to my advisor Dr. Kenneth Brezinsky for giving me the opportunity to carry out research in his laboratory at University of Illinois at Chicago. His guidance at every step of my research has facilitated a timely completion of this research with successful results.

I would like to thank my thesis committee – Dr. Kenneth Brezinsky, Dr. Robert Simon Tranter and Dr. Patrick Lynch for agreeing to be a part of my thesis committee. The guidance and assistance provided by them in every hurdle during my research helped me successfully overcome the hurdles and achieve my research goal. I would also like to thank the Army Research Office (ARO) for their funding to carry out this research through grant no. W911NF-16-1-0063.

I am thankful to my lab mates and members of the *UIC - High Pressure Shock Tube Lab*, Miroslaw Liszka, Xu Han and Juan Guzman who helped me tackle various problems I faced during the course of my research. Without their support and guidance, the research would be incomplete.

Lastly, I want to thank my family back home for their unconditional support and encouragement to pursue the path of research, now and in future.

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LIST OF ABBREVIATIONS

UIC	University of Illinois at Chicago
HPST	High Pressure Shock Tube
GC	Gas Chromatography
TFE	1,1,1 trifluoroethane
CPCN	Cyclopropyl Cyanide
DAQ	Data Acquisition System
FID	Flame Ionization Detector
ms	Milliseconds
К	degree Kelvin
atm	atmosphere
psi	Pound per square inch
ppm	Parts per million
MW	Molecular weight
in	Inches
Ar	Argon
Не	Helium
NI	National Instruments Corporation
РСВ	PCB Piezoelectronics, Inc.
L	Liters
HiPCO	High Pressure Company

NOMENCLATURE

- Pi Pressure
- T_i Temperature
- M_i Mach number
- ai Speed of sound
- R_i Specific gas constant
- γ_i Ratio of specific heats
- A_i Cross sectional area
- D_i/ϕ Diameter
- t Time
- ui Speed
- ρ_i Density

SUMMARY

A shock tube is one of the most prominent experimental devices used for studies in various fields of engineering. It plays a key role in the study of chemical kinetics, gas dynamics and ignition times. It allows generation of extremely high temperatures and pressures for various dwell times allowing for study of several types of combustion reactions for hydrocarbon fuels. Pyrolysis and oxidation studies of hydrocarbons are widely carried out in shock tubes.

The chemical kinetics of the reactions depend upon the pressure and temperature conditions within the shock tube's reaction zone which under normal operation do not remain constant over the reaction time. This adds to uncertainties in the experimental data. Thus, methods need to be employed for optimizing the characteristics in the reaction zone so they are close to ideal values allowing for analysis with lower uncertainties.

Methods to compensate for non-ideal effects and to prevent phenomena such as contact surface interaction are described for use in a small bore high pressure shock tube. The methods are experimentally tested and a close to ideal performance was obtained in the post shock region. The reaction time was also improved using back-filling of the driver section with a gas having low speed of sound. This technique increased the reaction time by as much as 4 times that of the regular method with no physical modifications to the shock tube.

The methods in combination were used with a temperature calibration for the shock tube using two chemical thermometers. Calibrations curves were obtained for a temperature range from 900 K to 1350 K. The calibration showed a high level of agreement between the calibrated temperature and the ideal temperature calculated using ideal shock tube theory.

1 INTRODUCTION

1.1 Background

A shock tube is a device in which a normal shock is produced in a test gas to instantaneously raise the pressure and temperature of the test gas for a fixed amount of time. The effect of the rise on the test gas can be studied using optical and quantitative methods, such as gas chromatography. The test gas is often a very dilute mixture of a fuel to be tested in an inert gas. Chemically kinetic studies can be carried out on the fuel and reaction mechanisms can be obtained.

The shock is formed by suddenly exposing two zones having very high-pressure difference instantaneously to each other using a diaphragm which separates the two sections and ruptures at the required pressure difference. This sudden pressure discontinuity in the tube causes a very fast shock to travel towards the driven section end wall and reflect off it. The driven section is the section of the shock tube with the lower pressure and is filled with the test gas. The driver is the high-pressure gas region which causes the diaphragm to burst and forms the subsequent shock. Driver gas is usually an inert gas with no fuel present in it.

The shock formed travelling towards the driven end wall is called the incident shock and it raises the temperature and pressure of the test gas. The shock when reflected off of the end-wall forms the reflected shock, behind which the pressure and temperature further increase to very high values. It is this region that is used as the test region. The time for which the pressure is maintained in this region depends on the time taken for the driver expansion wave to arrive and quench the reflected shock.

While the shock or compression wave is formed in the driven region because of diaphragm opening, an expansion wave travels towards the driver end wall. This expansion wave reflects off the driver end wall and travels towards the reflected shock wave. The interaction between the reflected driver expansion wave and reflected shock wave causes the shock to quench and the tube gradually reaches a lower pressure. The time for which the reactions occur depend upon the difference in the time at which the shock reflects and the time at which the expansion waves and reflected shock meet.

As seen in Figure 1, it is usual to denote the initial conditions in the driven section by subscript 1 and initial conditions in driver section by subscript 4. The driven section region behind the incident shock wave is denoted with subscript 2 and subscript 5 is used for driven section region behind the reflected shock wave. The subscript 3 is used to denote the cold flow

region which is the region at the tail of the driver expansion wave. The subscript 's' is used to denote incident shock and subscript 'r' denotes the reflected shock.



Figure 1 Pressure and Temperature distribution in a shock tube post incident shock reflection. Adapted from 'Modern Compressible Flow with Historic Perspective by John D. Anderson'[1]

1.1.1 IDEAL SHOCK TUBE THEORY

Ideal shock tube theory provides a simple model of a shock tube assuming isentropic conditions in the expansion region and no mixing regions in the shock tube, despite different driver and driven gases. The shock is treated as a discontinuity. It relates all the region in the shock tube, pre and post incident shock reflection and is used to calculate ideal operating conditions of a shock tube for the required reaction region pressure and temperature. The relations based on this theory are well known and published [1][2].

The region across the incident shock is related to the incident shock wave Mach number based on normal shock theory,

$$\frac{P_1}{P_2} = \frac{2\gamma_1 M_s - (\gamma_1 - 1)}{\gamma_1 + 1}$$

$$= \frac{\left(\gamma_1 M_s^2 - \frac{(\gamma_1 - 1)}{2}\right) \left(\frac{(\gamma_1 - 1)}{2} \cdot M_s^2 + 1\right)}{\left(\frac{\gamma_1 + 1}{2}\right)^2 \cdot M_s^2}$$
1.2

The region across the expansion wave is directly related using the isentropic relations,

 $\frac{T_1}{T_2}$

$$\frac{P_3}{P_4} = \left(\frac{T_3}{T_4}\right)^{\frac{\gamma_4}{\gamma_4 - 1}} = \left[1 - \frac{\gamma_4 - 1}{2} \left(\frac{u_3}{a_4}\right)\right]^{\frac{2\gamma_4}{\gamma_4 - 1}}$$

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The ideal shock tube theory also assumes an infinitely small contact surface between two gases, with no mixing of gases from driver and driven region. This contact surface ideally would be invisible to the reflected shock and it will pass right through it.

The driver and driven pressure is also related to each other directly by[3],

$$\frac{P_4}{P_1} = \frac{\left[\frac{2\gamma_1 M_s^2 - (\gamma_1 - 1)}{\gamma_1 + 1}\right]}{\left[1 - \frac{\gamma_4 - 1}{\gamma_1 + 1} \cdot \frac{a_1}{a_4} \left(M_s - \frac{1}{M_s}\right)\right]^{-\frac{\gamma_4}{\gamma_4 - 1}}}$$

The strength of the shock is primarily dependent on the ratio of speeds of sound in the driver and driven region. The speed of sound is give as,

$$a_i = \sqrt{\gamma_i \cdot \frac{R}{MW_i} T_i}$$

1.5

Where, R is the universal gas constant, 8.3144598 $\frac{J}{mol.K}$,

Further the reaction region properties are related to the initial driver conditions directly, based on the incident shock Mach number,[2]

$$\frac{T_5}{T_1} = \frac{[2(\gamma_1 - 1)M_s^2 + (3 - \gamma_1)][(3\gamma_1 - 1)M_s^2 - 2(\gamma_1 - 1)]}{(\gamma_1 + 1)^2 M_s^2}$$

1.6

$$\frac{P_5}{P_1} = \left[\frac{2\gamma_1 M_s^2 - (\gamma_1 - 1)}{\gamma_1 + 1}\right] \left[\frac{(3\gamma_1 - 1)M_s^2 - 2(\gamma_1 - 1)}{(\gamma_1 - 1)M_s^2 + 2}\right]$$

1.7

The speed of sound depends on the molecular weight of the gases used, as seen in equation 1.5. The shock strength controls the temperature that can be obtained behind the reflected shock. The ratio of speed of sound in the driven gas and driver gas is proportional to the shock strength. To attain the greatest speed of sound ratio of driven gas over driver gas, the molecular weight of the driven gas should be much higher than that of the driver gas. For this reason, the common gases used in driven section are helium (He) and hydrogen (H₂). The driven section gases are selected from the heavier inert gases like argon (Ar), xenon (Xe), neon(Ne) and krypton (Kr). Other gases that can be used in driven sections include nitrogen (N₂), carbon dioxide (CO₂) and Air.

1.2 Motivation

The UIC- High Pressure Shock Tube (HPST) is used to carry out chemical kinetic studies of fuels such as biodiesels, diesels, jet fuels, marine fuels and rocket propellants. These studies greatly depend on achieving very high pressure and temperature instantaneously to develop a combustion like atmosphere over a desired amount of time. The shock tube is advantageous for these studies as it generates the required conditions in the reaction zone instantaneously and quickly quenches the zone, thereby freezing the chemistry after the desired amount of time.

The UIC-HPST has an operating range from 15 atm to 1000 atm, with 600K to 2000K temperature range. The shock tube is designed to sustain the test conditions in the reaction region for 0.5 ms to 2.0 ms. The performance of the shock tube within these ranges over the designed reaction time can be close to ideal as seen in Figure 2, where in the region properties are maintained relatively constant.

Current projects at UIC - Shock Tube Laboratory, require analysis of chemical kinetics of low cetane number fuels at low temperatures and high pressures. Temperatures of 700 K – 1000 K with pressure ranging from 50 atm to 300 atm are needed to carry out these studies. The lower temperatures require a longer reaction time, as high as 10ms for the fuel to react. This requires holding pressure and temperature constant in the reaction region for time periods beyond the designed time periods of the shock tube.



Figure 2 High pressure test shock at 830 atm , lasting almost constantly over 1.2 ms [3].

The increase in reaction time can cause non-ideal and unwanted phenomena in the shock tube. The most prevalent phenomenon observed is the interaction of the reflected shock with the contact surface formed at the interface of the driver and driven gases. This interaction results in several outcomes. The outcomes cause the pressure and temperature in the reaction region to change, often drastically. This drastic unwanted change interferes with the chemical kinetics of the fuel and can yield uncertain results.

The non-ideal pressure rise behind the reflected shock wave due to boundary layer effects, shock attenuation, diaphragm opening and several unknown reasons also become very prominent. These effects need to be eliminated or minimized below acceptable levels to carry out accurate chemical kinetic studies.

This thesis deals with several methods that have been employed to obtain the required close to ideal constant pressure conditions, as seen in Figure 3, which is expected to lead to a constant temperature in the reaction region.



Figure 3 Shocks with similar conditions to show the effect of tailoring of the driver gas and use of a driver insert resulting in the optimized shock.

2 HIGH PRESSURE SHOCK-TUBE

2.1 Overview[3]

The High-Pressure Shock Tube at University of Illinois at Chicago is a single pulse high pressure shock tube capable of developing reaction region pressures up to 1000 atm with temperatures ranging to 2000K easily. It is designed for ideal operation over reaction times up to 2 ms, which sufficiently permit the investigation of hydrocarbon oxidation and pyrolysis reactions. The construction of the shock tube permits increasing the driven section length and reducing the driver section length, so that required reaction time can be achieved with constant reaction region conditions.

The UIC- HPST is manufactured using single 17-4PH stainless steel billet to prevent welding. By using a single turned and bored billet, close tolerances can be maintained between various mating parts and improves alignment between all sections. The bore has a tolerance of ± 0.002 inch and drift of ± 0.001 inch. The high pressure and temperature range to which the tube is exposed, can be better handled by a single machined tube over welded tubes.

The shock tube is heated to 373 K throughout to prevent condensation of the fuel in the test gas. Coil heaters and PID controllers with K-Type thermocouples are used to maintain the shock tube at this temperature.



Figure 4 Overview of the UIC-High Pressure Shock Tube[4]

The length of the shock tube directly controls the reaction times obtained post-shock. The UIC-HPST has provisions for changing its length, so that required reaction times can be obtained. The driver section length is 60 inches and can be reduced to reduce the required reaction time by using solid plugs inside the shock tube. To increase the reaction time, the driven length can be increased. The UIC-HPST has a minimum driven length of 120 inches. Two extensions are available, 20 inches and 40 inches long which can increase the driven section length up to 160 inches to gain longer reaction times.

UIC-HPST is a convergent shock tube having a driver diameter of 2 inches and the driven diameter of 1 inch, with a convergent section at the diaphragm section. This design allows developing a higher post-shock pressure for the same initial driver and driven pressures. The shock tube can be run as a constant bore tube by using an insert in the driver section, which reduces the diameter of the driver section of the shock tube to 1 inch. This helps in conserving gas when running the shock tube for low reaction pressures and helps eliminate some unwanted phenomenon observed in a convergent shock tube for specific operating conditions.

2.2 Ancillary equipment[3]

2.2.1 HIGH PRESSURE CYLINDERS

The driver needs to be loaded to pressures as high as 8,000 psi, to achieve reaction region pressures of about 5,000 psi or 300 atm. This high loading pressure cannot be achieved using the commercial compressed gas cylinders available since they have maximum pressure of 2,500 psi when full. This would mean that even one cylinder will not be sufficient to fire one shock. To remedy this, ten high pressure cylinders made of solid steel, having a volume of 6.5 L each are used to store pressurized gases, used in the driver of the shock tube. The gases are boosted to pressures of up to 13,500 psi using a compressed air driven booster pump and stored in the high-pressure cylinders. The cylinders are fitted with blow off valves to prevent over-pressurization. The cylinders are connected in groups of 5 cylinders, so that one bank can be used to fire shocks while the other bank is being boosted. Typically, one bank of cylinders boosted to 6,000 psi can give about 30 shocks having post shock pressures of 750 psi.

2.2.2 DRIVER DIAMETER REDUCING INSERT

The insert used to reduce the driver diameter to 1 inch from 2 inches is made of solid carbon steel, having an outer diameter of 2 inches and a through bore of 1 inch is shown in Figure 5. The length of the insert is the same as that of the driver section and lines up within the driver section exactly. The side of the insert towards the diaphragm has a taper on the outer diameter which mates with the convergent section before the driver. Groove and ports are provided to carry out the filling of the inside bore, which is effectively the driver section.





Figure 5 Driver diameter reducing insert



Figure 6 Modified driver diameter reducing insert

The driver diameter reducing insert was extremely heavy and had warped since its long length and high mass deformed it with time. The material used for the insert is plain carbon steel which is highly susceptible to corrosion which added to this problem. The insert was unable to freely slide into the shock tube due to the deformation and warpage and had to be modified.

Due to warpage the insertion of the insert into the shock tube driver could score the internal bore of the driver section. The driver bore reducing insert had an outer diameter of 2 inches which was turned down to 1.6 inches to prevent damaging the driver section bore while insertion. Two collars of 2 inches and 1.5 inches were kept with a 2-inch diameter at the beginning and end of the insert respectively. This was done to ensure that the driver and driven bores aligned correctly. Two more ¾ inch long collars were kept on either side of the driver gas filling port to support the insert and prevent bending. This modification reduced the mass of the insert making it easier to handle and store. A drawing of the modified insert is shown in Figure 6.

2.2.3 VALVES

Since the operating pressures of the HPST can go as high as 15,000 psi, high pressure valves having a rating of at least 20,000 psi from HiPCO are used. The manually operated valves to control gas delivery to and from the shock tube and to the high-pressure cylinders described in section 2.2.1 are HiPCO – 20-11LF4 valves, which have maximum operating pressure of 20,000 psi and use ¼" HiPCO high pressure connections. The automatic valves used to fill the shock tube for firing and to carry out sampling of post shock test gas are pneumatically operated, solenoid-controlled valves (HiPCO – 20-11LF4-NC). Additionally, metered valves are used to maintain near constant fill rate to the driver and driven section, irrespective of the source cylinder pressure. The HiPCO - 60-11HF4-V valves are used for the metering purpose and have operating pressure range up to 60,000 psi.

2.2.4 PRESSURE GAUGES

Several pressure gauges are used in the complete apparatus to monitor and control the operation of the shock tube. Process gauges having a range of 20,000 psi, of 6-inch diameter are used to measure the cylinder pressure for each high-pressure cylinder. Driver and driven sections are equipped with DCT - JA series pressure gauges, which give a digital read out and transmit the reading to the shock tube control system. The vacuum in the driven section is measured by a Lesker – KJL902006 pressure transducers.

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2.2.5 DIAPHRAGMS

The driver and driven sections are separated by a diaphragm, which when removed instantaneously forms a shock as a result of the pressure differential between the two sections. The loading pressure of the driver depends on the choice of diaphragm size and material. The higher the driver to driven pressure ration, the stronger will be the shock, developing higher pressure in the reaction region. This implies that the size of the diaphragms directly relates to the required reaction region pressure. Pre-scored metal diaphragms of varying thickness are used to achieve the required pressure in the reaction region. The diaphragms are pre-scored to ensure clean opening of the diaphragms into 4-petal like structures as seen in Figure 7 and Figure 8. The burst pressure is not just the function of the diaphragm thickness but also of the depth of the score on the diaphragm. The materials used for diaphragms are brass and aluminum.

Diaphragm Thickness (inch)	Material	Average Pressure (P5) [atm]	Score Depth (inch)	Temperature Range (T5)[K]
	Aluminum		0.008″	1300-1600
0.025″		20	0.009"	1000-1300
			0.010"	700-1000
	Aluminum	60	0.004"	1300-1600
0.032"			0.005″	1000-1300
			0.006"	700-1000
0.049"	Aluminum	120	0.004"	1200-1600
0.048		150	0.0045″	700-1200
		125	- 0.006" - 0.008"	700-1100
		100		1100-1500
		100		700-1100
		80		1100-1500
	Brass	50	0.010"	1100-1500
		40	0.012"	700-1100
0.020"		35		1100-1500
0.020		35	0.013"	700-1100
		30		1100-1500
		30	0.014"	700-1100
		25		1100-1500
		25		700-1100
		<20	0.015	1100-1500
		15-20	0.016"	1100-1600

Table 1 Various dimensions of the diaphragms currently used in the UIC-HPST (dimensions are found experimentally)

The diaphragm specifications provided in the Table 1 are currently used to obtain the required reaction region conditions. The values of reaction region conditions obtained with these diaphragm is applicable to shocks fired using the various techniques described in this thesis.

The values for the reaction region pressure are tested for the convergent configuration of the shock tube, when the area ratio, A_4/A_1 is 4. When the shock tube is run with constant driver and driven diameters the pressure in the reaction region for every diaphragm is reduced. The reduction in pressures is exponential and not linear, thus the variation for lower pressure shocks is negligible while it is highly evident at high pressure shocks.



Figure 7 Representational aluminum diaphragm used in UIC-HPST. Post Shock (left), Pre-shock(right).



Figure 8 Representational soft brass diaphragm used in UIC-HPST. Post Shock (left), Pre-shock(right).

2.3 Data Acquisition and Control System[3]

The software used to control the shock tube operation and to carry out DAQ is written using LabVIEW 2009. The pneumatic valves that control the filling of the shock tube sections and carry out sampling are controlled by the software. The software controls low voltage relays through National Instruments DIO-24 card, which in turn operate high voltage relays which control the flow of air to the pneumatically operated HiPCO – high pressure valves described in section 2.2.3. The sequence of opening is programed in the software so that the steps required for firing shocks are synchronized to maintain high accuracy. The software reads pressure in the driver and driven section through the DCT – JA Series pressure gauges through National Instruments PCI-MIO-16-E-1 card.

The transducer section, which is the primary test section has provisions to connect 9 pressure transducers, of which 8 are on the side wall and 1 on the end wall, to measure the pressure right at the end-wall. The primary purpose of the side-wall transducers is to measure the velocity of the incident shock wave to compute the expected ideal temperature. The shock velocity is measured by using the difference in time for the wave to travel between two transducers and extrapolated over time differences from all transducers. The shock tube currently uses 7 pressure transducers, with location 1 and 6 plugged. PCB Electronics 113A23 series transducers are used, which have operating range of up to 10,000 psi. The output from the transducer is conditioned using a PCB Electronics 482A20 – Power Supply and Signal Conditioner. The conditioned signal, after voltage reduction is read by ComputerBoards DAS-4020 card. This signal can be read at rates as high as 20MHz. Two boards, each having 4 digital channels are used to acquire transducer data from the transducer section.

LabVIEW is used to interpret and plot the data acquired from the pressure transducers. The DAQ software also provides the reaction time and the time intervals at which the shock arrived at the pressure transducers. The interface for the program showing the end wall pressure trace for a low temperature-tailored shock can be seen in Figure 9.



Figure 9 Interface of in-house developed Data Acquisition Program

2.4 Sampling System and Analytical Techniques

The shocked gas sample from the shock tube is studied using gas chromatography after the reflected shock. An online gas sampling system is used [4], where the sample is directly extracted from the shock tube after reflection of the shock, into the sampling loops of the GC and the GC analysis is carried out while the shock tube prepares for the next shock.



Figure 10 Schematics of the sampling system

The HPST is connected to two, Agilent Technologies – 7890B GCs, equipped with FID and TCD. The first GC is equipped with two FIDs and the second one has a combination of FID and TCD. The columns used for analysis with all four detectors are different so that all species can be captured from the test gas sample. The sampling lines are evacuated using a separate vacuum pump so that they can be maintained under constant vacuum, even during shock tube operation. A capacitance manometer is used to measure the pressure in the sampling line to a value as low as 0.001 psi. The sample is injected into the GC when it reaches a stable pressure. The Agilent Technologies 7890B GCs use pneumatically operated automatic injection valves so the delay between the GC method start and sample injection is negligible.

A buffer vessel is used between the shock tube and the GCs to prevent over pressurization of GC lines due to high pressure in the shock tube. The sampling lines are coated stainless steel lines provided by Restek with a coating claimed to provide inert performance, preventing absorption of any species while the gas sample travels through the sampling lines. The sampling line from sampling value to the GC through the buffer vessel and the line connecting the GCs to each other and the capacitance manometer are of ½ inch diameter whereas the line between the GC valves and sample loops are of ¹/₁₆-inch diameter. Small internal diameter lines are used to increase the surface area to volume ratio. This ensures the sample is thoroughly heated and no condensation of species occurs in the lines. It also helps in ensuring constant pressure drop along the flow path. The complete sampling system, from the sampling valve to the exhaust is heated to a temperature of 423 K to ensure no species undergoes condensation within the sampling line.

Provisions are provided to flush the GC lines with helium post analysis to make sure the next sample is not affected by the previous. The lines are flushed repeatedly after each run and pumped down to completely avoid mixing of test gas from two experiments.

3 DRIVER GAS TAILORING

3.1 Need for Gas Tailoring

The single pulse shock tube utilizes the region behind the shock reflected by the driven section end-wall to carry-out pyrolysis or oxidation studies of hydrocarbon fuels. The region should hold nearly constant temperature and pressure for the required reaction time to achieve best results. The breakdown of the fuel in these reactions is greatly affected by the pressure and temperature conditions observed in the reaction region. The ideal approximation of the pressure and temperature made using ideal shock relations cannot be directly achieved due to non-idealities in the shock tube. One of the non-idealities observed in shock tubes is interaction with the contact surface which does not allow the reflected shock to pass through it with no effect to the shock.

This contact surface often interferes with the reflected shock and produces several conditions which affect the pressure and temperature in the reaction region to not just deviate from ideal but to also not remain constant throughout the reaction period. The effect of contact surface interaction of the shock wave on the pressure in the region behind reflected shock can be seen in Figure 11.



Figure 11 Pressure trace from the end wall transducer showing the effect of interaction of shock and contact surface, resulting in the pressure bump.

3.1.1 REFLECTED SHOCK PASSES THROUGH THE CONTACT SURFACE

This is the Ideal case wherein the reflected shock passes through the contact surface as if it is non-existent. This behavior is necessary to avoid inconsistency in the temperature and pressure in the reaction region. Figure 12 illustrates this behavior schematically. This is the desired case and for it to occur [5].



$$\frac{a_3}{\gamma_3-1} = \frac{a_2}{\gamma_2-1}$$

Figure 12 x-t diagram for shock wave passing through the contact surface

3.1.2 REFLECTED SHOCK REFLECTS FROM THE CONTACT SURFACE TOWARDS THE ENDWALL

This case resembles the most common and unwanted behavior observed in shock tubes. The shock reflected from the contact surfaces causes a sudden rise in the pressure and temperature in the reaction region, making the conditions highly non-ideal. In adverse situations repeated shocks resonate between end-wall and the contact surface causing a severe rise in the gas properties in that region. The Figure 13 shows the schematics of this phenomenon in a shock tube. This occurs in the shock tube when the following condition holds true for the shock tube,

$$\frac{a_3}{\gamma_3-1} < \frac{a_2}{\gamma_2-1}$$



Figure 13 x-t diagram for shock reflecting from the contact surface

3.1.3 REFLECTED SHOCK CAUSES AN EXPANSION WAVE OFF THE CONTACT SURFACE[5]

The case where the contact surface reflects an expansion wave instead of a shock is rare and is difficult to achieve. This case is often used to improve the quenching rate in reaction region. Premature formation of an expansion wave from interaction with the contact surface shortens the reaction time an interferes with the progress of the reactions to be observed. The schematic is shown in the. The condition occurs in a shock tube only when following conditions are observed[5], [6]

$$\frac{a_3}{\gamma_3-1} > \frac{a_2}{\gamma_2-1}$$



Figure 14 x-t diagram for expansion wave reflecting from the contact surface

The Microsoft excel sheet shown in Appendix C can be used to calculate the ideal condition in the shock tube based on initial conditions used to generate the shock. The sheet also compares the impedance condition present across region 2 and 3 in the shock tube for the particular shock based on which the interaction between the discontinuity and the reflected shock can be known.

In a single pulse shock tube to improve the quenching rate, its desirable to have an expansion wave reflect off the contact surface as explained in section 3.1.3 and illustrated in Figure 14 which can be achieved by obtaining greater acoustic impedance in region 3 than region 2. The driver gas used has a much lower molecular weight than the driven gas which maintains higher impedance in region 3 than region 2. However, when longer reaction times are observed the expansion wave reflected from the contact discontinuity reflects again from the driven end-wall as an expansion wave and interacts with the contact surface discontinuity forming a compression wave travelling in the reaction region towards the driven end-wall which gradually raises the pressure in the reaction region. This is observed in the form of a pressure hump in the reaction region. The occurrence of this phenomenon was observed by Klepeis[6] through experiments.

To avoid the occurrence of this pressure bump, we need to eliminate the interaction of the reflected shock with the contact discontinuity. If there is no interaction of the reflected shock and the contact surface discontinuity, no secondary wave will be formed in the reaction region causing pressure variations. To achieve this the tailoring of the driver gas is carried out by mixing two or more gases in calculated proportion for matching acoustic impedance in region 2 and 3.

3.2 Tailoring of Driver Gas

The method used to tailor the driving gas is based on the steps from Hong et al [7]. The objective is to match the acoustic impedance in the regions 2 and 3[8], so that the reflected shock wave passes through with no obstruction and hence does not reflect. Since the ratio of specific heats is same for the driver and driven gas ,the required condition mathematically is,

$$a_2 = a_3$$

3.1

Since the temperatures in the region 2 and 3 are defined by the incident shock and driver expansion wave, the only parameters that can be altered is the molecular weight and the ratio of specific heats which depends on the choice of the driver and driven gas. The tailoring is carried out by mixing gases in the driver section so that the effective specific molecular weight and ratio of heat capacities result in pressure in region 3 equal to that in region 2. The effective molecular weight and the ratio of heat capacities for a gas mixture is calculated based on following relations.[2]

$$\gamma = \sum_{i} \frac{\frac{x_i \gamma_i}{\gamma_i - 1}}{\sum_i \frac{x_i \gamma_i}{\gamma_i - 1} - 1}$$
Molecular Weight (MW) = $\sum_i x_i MW_i$

3.2

Where γ_i represents the ratio of specific heats for each gas, x_i represents the fraction of each gas and MW_i is the molecular weight of each gas in the mixture.

The ideal properties in each zone in the shock tube can be calculated for the desired conditions using the standard one dimensional normal shock relations for a shock tube developed as follows [2]

$$\frac{T_5}{T_1} = \frac{[2(\gamma - 1)M_s^2 + (3 - \gamma)][(3\gamma - 1)M_s^2 - 2(\gamma - 1)]}{(\gamma + 1)^2 M_s^2}$$

The above equation can be used to calculate required shock Mach number (M_5) for the desired temperature (T_5), which can be used to calculate the required driven pressure (P_1) needed to obtain the pressure (P_5) in the reaction region.

$$\frac{P_5}{P_1} = \left[\frac{2\gamma M_s^2 - (\gamma - 1)}{\gamma + 1}\right] \left[\frac{(3\gamma - 1)M_s^2 - 2(\gamma - 1)}{(\gamma - 1)M_s^2 + 2}\right]$$

3.4

3.3

The local speed of gas in the region behind shock can be found using,

$$u_2=\frac{2a_1}{\gamma+1}(M_s-\frac{1}{M_s})$$

3.5

And pressure (P₂) behind the incident shock wave is given by[2]

$$\frac{P_2}{P_1} = \frac{2\gamma M_s^2 - (\gamma - 1)}{\gamma + 1}$$

3.6

$$\frac{P_5}{P_2} = \frac{\frac{\gamma+1}{\gamma-1} + 2 - \frac{P_1}{P_2}}{1 + \frac{\gamma+1}{\gamma-1} \cdot \frac{P_1}{P_2}}$$

3.7

In tailored case the following relation provided by Nishida[8] holds true and can be used to compute speed of sound (a₃) in region 3,

$$a_{3} = u_{2} \frac{\sqrt{\left(1 + \frac{\gamma + 1}{\gamma - 1}\right)\left(1 + \frac{\gamma + 1}{\gamma - 1} \cdot \frac{P_{5}}{P_{2}}\right)}}{\left(\frac{\gamma + 1}{\gamma - 1} - 1\right)\left(\frac{P_{5}}{P_{2}} - 1\right)}$$

Applying characteristic equations across the expansion wave[1],

$$\frac{a_3}{a_4} = 1 - \frac{\gamma - 1}{2} \left(\frac{u_3}{a_4} \right)$$

-		
- 2		0
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3.8

we can get the required speed of sound in the driver section (a4) to achieve the tailored condition. The speed of sound relation can be used to calculate the required average molar weight (MW4).

$$\frac{a_4^2}{\gamma T_4} = \frac{R}{MW_4}$$

3.10

Where, R is the universal gas constant, 8.3144598 $\frac{J}{mol.K}$

$$x_{He} + x_{Ar} = 1$$
$$MW_{He}x_{He} + MW_{Ar}x_{Ar} = MW_{Ar}$$

3.11

Where x is the mole fraction of each gas, MW is the known molecular weight of each gas and MW₄ is the required average molecular weight in the expansion.

For the desired values of T_5 and P_5 , using the known value of T_1 , we can calculate properties in all other regions. To achieve the same speed of sound in region 2 and 3 the alteration of driver gas mix is carried out allowing this condition.

3.3 Driver Gas Tailoring for UIC – High Pressure Shock Tube

3.3.1 CONVENTIONAL TUBE: DRIVER $\phi 1^{"}$ – DRIVEN $\phi 1^{"}$

The ideal relations directly apply to the calculation of ideal values of temperature and pressure in each region. The UIC – High Pressure Shock Tube (HPST) is heated and maintained at 373 K and is the initial temperature of driven section (T_1) and driver section (T_4). An Excel spread sheet as shown in Appendix B is used to compute the ideal conditions for the required pressure (P_5) and temperature (T_5) in the reaction region as input. The procedure is as follows:

- 1. The properties behind the incident shock and across the contact surface are obtained using equations 3.5 and 3.6.
- Using the properties calculated behind the shock and the pressure ratio across reflected shock from equation 3.7, we can compute the required speed of sound in the cold flow region 3 for tailored conditions by equation 3.8.
- 3. Since the temperature in the cold flow region cannot be measured, we can use equation 3.9 to compute the required speed of sound in the driver gas as the velocities of gas in region 2 and 3 are equal.
- 4. Equations 3.10 and 3.11 can then be used to compute the required gas composition for tailored driver gas.

The UIC – HPST uses argon and helium as the primary driven and driver gas respectively. This further simplifies the calculation of the mixture ratio as both these gases have same value for specific heat capacities γ . The ratio of mixing does not affect the value of the heat ratio. This makes the tailoring ratio, just the function of the molecular weights of the mixed gases to achieve the tailoring conditions. Simultaneous solution of following two equations allows computation of the required mixing ratio.

The effect of tailoring the driver gas can be seen by the constant pressure region observed in the end wall pressure trace of a shock shown in Figure 15. The mixing ratio for the driver gas for tailoring was found to deviate from the calculated values when experimentally tested. The values found by calculation when used provided very little or no effect on the occurrence of the contact surface interaction. Experimentally found values which provide the best results for a given temperature range have been shown in Table 2.


Figure 15 End wall transducer read out for a test shock profile for a tailored driver gas at a nominal pressure of 42 atm and 1240.26K ideal temperature with eliminated pressure rise bump due to contact surface interaction.

Temperature (K)	%Ar (as calculated)	%Ar (experimentally used)
800	0.343512916	34-38
900	0.278301114	_
1000	0.226150122	
1100	0.180186004	29-33
1200	0.143609934	
1300	0.111128563	24-28
1400	0.082335015	

Table 2 Comparison of Experimental and Theoretical Driver Gas Tailoring Conditions for a conventional Tube (% Ar in He)

3.3.2 CONVERGENT TUBE: DRIVER $\Phi 2'' - DRIVEN \Phi 1''$

The tailoring conditions vary depending not just on the required temperature and pressure but also on the physical characteristics of the shock tube. In a convergent shock tube, the required initial driver pressure is lower than that in a conventional tube to achieve the same pressure in the reaction zone. This has been explained by Alpher and White[9]. It also connects the incident Mach number M_s with the Mach numbers in the convergent section; M_t, M_{3a} and M₃. Resler et al [10] uses theses relations to compute an equivalence factor 'g' which relates the driver pressures of two equivalent shock tubes

with and without convergent section for the same pressure behind the reflected shock. This relation helps relate driver gas tailoring in a conventional tube to a convergent tube and is explained in detail by Hong et al [7].



Figure 16 Instantaneous pressure distribution before shock reflection in a convergent shock tube. Adapted from Alpher and White[9]

In case of a convergent tube the properties of the region 3 cannot be directly deduced from the one-dimensional isentropic shock tube relations as the effective properties - M₃, P₃ and T₃ in that region depend greatly on the effect of area reduction because of the convergent section. As seen in the Figure 16 the convergent section develops more regions within the shock tube namely 3a and 't' which are explained by Alpher and White [9]. At the exit of the convergent section a secondary expansion may be formed as a result of the convergent section if the flow in the region is not sub sonic. This requires additional isentropic relations to relate the region 3 with region 't'. Absence of this expansion wave results in the properties being constant in the region 't' and 3. Thus, the properties of these region need to be calculated keeping in mind the effect of area change using the well-known Mach number-area relation.

The driver to driven area ratio is related to the Mach numbers at the convergent location by the following equations given by Alpher and White[9],

$$\frac{A_4}{A_1} = \frac{M_t}{M_{3a}} \cdot \left[\frac{2 + (\gamma_4 - 1)M_{3a}^2}{2 + (\gamma_4 - 1)M_t^2} \right]^{\frac{(\gamma_4 + 1)}{2(\gamma_4 - 1)}}$$

and,

$$M_3 = \left(\frac{a_1}{u_2}, \frac{a_4}{a_1}, g^{\frac{\gamma_{4-1}}{2\gamma_4}} - \frac{\gamma_{4-1}}{2}\right)^{-1}$$

3.13

3.12

Where, the equivalence ratio 'g' is given by[10],

$$g = \left\{ \sqrt{\frac{2 + (\gamma_4 - 1)M_{3a}^2}{2 + (\gamma_4 - 1)M_t^2}} \cdot \left[\frac{2 + (\gamma_4 - 1)M_t}{2 + (\gamma_4 - 1)M_{3a}} \right] \right\}^{\frac{2\gamma_4}{(\gamma_4 - 1)}}$$

Since the UIC – High Pressure Shock Tube is designed to operate with a subsonic cold flow region, the properties at the throat of the convergent section is same as the cold region in the driven section,

$$M_3 = M_t$$

3.15

3.14

The relation between incident shock Mach number and region 3 is given by [9],

$$M_{3} = \frac{\left(\frac{\gamma+1}{\gamma-1} - 1\right) \cdot \left(\frac{P_{5}}{P_{2}} - 1\right)}{\sqrt{\left(1 + \frac{\gamma+1}{\gamma-1}\right) \cdot \left(1 + \frac{\gamma+1}{\gamma-1} \cdot \frac{P_{5}}{P_{2}}\right)}}$$

5.10		3.	1	6
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With the equations above the speed of sound required in the driver gas can be calculated. The following steps should be followed to carry out tailoring of the driver gas.

- Calculate the Mach number in cold flow region 3 using equation 3.16, when the pressure ratios are known using equation 3.7 for the known shock Mach number
- Since equation 3.15 holds true in UIC-HPST , equation 3.12 can be used to iteratively find the Mach number in the region before the convergence (M_{3a}).
- 3. Using the known values of M_t and M_{3a} in equation 3.14, the equivalence ration 'g' can be found.
- 4. Equation 3.13 can now be solved iteratively to compute the speed pf sound required in the driver (a₄) using the calculated equivalence ratio. The velocity behind the shock wave can be computed with equation 3.5. The speed of sound in the driven section depends on the initial conditions of the driven section.

The required composition of gas can be determined using the required average molecular weight of the driver gas. It can be determined based on the required speed of sound in the driver region using equation 3.17,

$$\frac{a_4^2}{\gamma T_4} = \frac{R}{MW_4}$$

3.17

Where, R is the universal gas constant, 8.3144598 $\frac{J}{mol,K}$

$$x_{He} + x_{Ar} = 1$$
$$MW_{He}x_{He} + MW_{Ar}x_{Ar} = MW_4$$

3.11

Where x is the mole fraction of each gas, MW is the known molecular weight of each gas and MW₄ is the required average molecular weight in the driver.

The Microsoft Excel spreadsheet provided in Appendix B is used to iteratively solve for the required gas composition for the driver gas based on the method explained in the section 3.3.2. The input parameters needed are the required condition behind the reflected shock and the shock tube configuration. The choice of gases used in the shock tube are also an input parameter.

The effect of tailoring the driver gas can be seen by the constant pressure region observed in the end wall pressure trace of a shock shown in Figure 17. The mixing ratio for the driver gas for tailoring was found deviate from the calculated values when experimentally tested. The values found by calculation when used provided very little or no effect on the occurrence of the contact surface interaction. Experimentally found values which provide the best results for a given temperature range have been shown in Table 3.

Temperature (K)	%Ar (as calculated)	%Ar (experimentally used) 32.5-36		
800	0.366456755			
900	0.3343911			
1000	0.304205135			
1100	0.249427068	27-32.5		
1200	0.206059765			
1300	0.167618098	23-26		
1400	0.133379023			

Table 3 Comparison of Experimental and Theoretical Driver Gas Tailoring Conditions for a Convergent Tube (% Ar in He)



Figure 17 End-wall pressure transducer output for a test shock profile for a tailored driver gas at a nominal pressure of 58 atm and 1372.89K ideal temperature with eliminated pressure rise bump due to contact surface interaction.

4 COMPENSATION OF NON-IDEAL PRESSURE RISE USING DRIVER INSERT

4.1 Non-Idealities behind reflected shock wave

The temperature and pressure in the reaction region, which is the region behind the reflected shock, should remain constant until the shock is quenched, as shown by the ideal shock tube theory. However, in experimental situations this is often untrue. The pressure and temperature measured are often varying with respect to time and /or location as a result of non-ideal fluid behavior such as shock attenuation and boundary layer formation. The effect of non-idealities is especially prominent in shock tubes having a small bore [11]. The non-ideal behavior of pressure and temperature can also be attributed to the mechanics of the shock tube operation. The extent of diaphragm opening and diaphragm opening time often affect the shock formation which can cause non-ideal effects in the reaction region. Some studies also suggest that the rate of gas filling in the driver section affect the diaphragm opening behavior [11].As an example, the pressure profile for a test shock in the UIC- High Pressure Shock Tube in Figure 18 illustrates the effect of non-ideal behavior.

The non-ideal pressure rise can be characterized by The rate of pressure rise $\left(\frac{\Delta P_5^*}{\Delta t}\right)$ defined as the extent of pressure rise divided by the time required for rise where $\Delta P_5^* = \frac{P_5^{maximum} - P_5^{Start}}{P_2^{maximum}}$.[12]



Figure 18 Shock profile for a tailored driver gas showing the non-ideal pressure rise.

The effect of the non-idealities varies depending of the reaction region temperature and pressure, making it difficult to predict. The variation in temperature and pressure can cause uncertainties in chemical kinetic studies since the rate constants for several species are highly sensitive to temperature and pressure changes. This develops the need to reduce the effect of non-idealities in a shock tube for chemical kinetic studies.

4.2 Design of driver insert



Figure 19 Schematics of Driver Insert to compensate for non-ideal pressure rise

The non-ideal pressure rise can most effectively be prevented by incrementally partially reflecting the driver expansion wave before it completely reflects from the driver end wall as suggested by Hong et al [12]. This partial expansion wave compensates for the rise in the pressure in the reaction region without completely quenching the reflected shock. To do this a varying area insert was designed for the driver[12] which partially reflects the primary expansion wave towards the driven end-wall, preventing the pressure rise in the reaction region.

The insert as shown in Figure 19 is designed based on the divergent nozzle. The area characteristics of the driver with the insert can be considered equivalent to that of a divergent nozzle. The length over which area change is required is a direct function of the time over which the pressure in the reaction region rises. To calculate the area change required the shock tube model for a convergent tube given by Alpher & White [9] is utilized. By adjusting the relations between various regions, keeping in mind a diverging area instead of convergent area, Alpher and White's[9] relations can be used directly to arrive at the required area ratio for the given shock tube conditions.

4.2.1 LENGTH OF THE INSERT

The length of the insert required depends upon the expected reaction time. The time between the first partially reflected expansion wave and shock reaching the driven end-wall should essentially be zero so that the pressure rise is compensated completely. The x-t diagrams are plotted for the required driver and driven section conditions to obtain the desired reaction

region conditions. The length of the driver is reduced in steps to compute the x-t diagrams as shown in the Figure 20 till the reaction time obtained from the x-t diagram becomes zero as seen in Figure 21. The length of driver at which the reaction time becomes zero when subtracted from the actual driver length gives the required length of the insert.



Figure 20 x-t diagram obtained using the WiSTL Riemann Solver[13] for maximum reaction time



Figure 21 x-t diagram obtained using the WiSTL Riemann Solver[13] for zero reaction time

The x-t diagrams for various operating parameters over the general range of reaction times used in UIC-HPST were generated and an average length for the insert was fixed at 1.042 meters. This length was experimentally checked and found to have acceptable performance. The Riemann solver WiSTL [13] developed at University of Wisconsin was used to compute the x-t diagrams for various shock tube operating parameters.

4.2.2 LENGTH OF AREA CHANGE

The length of area change depends directly on the time over which the non-ideal pressure rise occurs and can be less than the total length of the insert. The time for pressure rise varies from shock to shock and is difficult to predict by calculations. Data from several experiments were combined to develop an average expected time for non-ideal pressure rise from which the length of area change was finalized. The average time for which non-ideal pressure rise occurs in the UIC-HPST is 0.75 ms. The insert is designed with possibilities for variation in area change length roughly centered at the average value.



Figure 22 Plot of driver length vs reaction time obtained using x-t diagrams

The required length is calculated using the slope of the line formed by the plot of reaction time against the driver length shown in Figure 22. The time over which the rise needs to be compensated when entered into the line equation (I = 16t + 24.8) for the graph in Figure 22 would give the required position in the driver at which the area change should end. The position found when subtracted from insert length would give the length of area change[12].

4.2.3 MAXIMUM DIAMETER OF THE INSERT

The rate of area change is the most important parameter of the driver insert and has the greatest effect on the performance of the insert. It is a function of the pressure rise in the reaction region. The area change required is calculated using the nozzle relations for a divergent nozzle such that the effective pressure variation across the area change will counter the pressure rise almost exactly to compensate for the unwanted pressure rise.

Alpher and White's theory [9] can now be used to calculate the divergent area ratio which will develop the required pressure deviation in the reaction region. An Excel sheet shown in Appendix C is used to calculate the required area ratio for various shocks.

The required driver pressure (P₄) is calculated for the reaction region pressure (P₅), when the initial temperatures and the required reaction region temperatures are known using the equation 4.1 [2].

$$\frac{P_4}{P_5} = \frac{\left[1 - \frac{\gamma_4 - 1}{\gamma_1 + 1} \cdot \frac{a_1}{a_4} \left(M_s - \frac{1}{M_s}\right)\right]^{-\frac{\gamma_4}{\gamma_4 - 1}}}{\left[\frac{(3\gamma - 1)M_s^2 - 2(\gamma - 1)}{(\gamma - 1)M_s^2 + 2}\right]}$$

4.1

The two driver pressures (P_{4s} and P_{4m}) can now be obtained from above equation for the minimum (P_{5s}) and maximum pressures (P_{5m}) observed in the reaction region respectively, for the measured Mach number.

$$\frac{P_{4s}}{P_{5s}} = \frac{\left[1 - \frac{\gamma_4 - 1}{\gamma_1 + 1} \cdot \frac{a_1}{a_4} \left(M_s - \frac{1}{M_s}\right)\right]^{-\frac{\gamma_4}{\gamma_4 - 1}}}{\left[\frac{(3\gamma - 1)M_s^2 - 2(\gamma - 1)}{(\gamma - 1)M_s^2 + 2}\right]}$$

$$\frac{P_{4m}}{P_{5m}} = \frac{\left[1 - \frac{\gamma_4 - 1}{\gamma_1 + 1} \cdot \frac{a_1}{a_4} \left(M_s - \frac{1}{M_s}\right)\right]^{-\frac{\gamma_4}{\gamma_4 - 1}}}{\left[\frac{(3\gamma - 1)M_s^2 - 2(\gamma - 1)}{(\gamma - 1)M_s^2 + 2}\right]}$$

$$4.2$$

ν.

This variation in driver pressure can be written in the form of 'equivalence ratio' as mentioned by Resler et al [10].

$$g=\frac{P_{4s}}{P_{4m}}$$

4.	4

4.3

The equivalence ratio can be used to calculate the required Mach number at the exit of the nozzle, which is region 3, using Alpher and White's theory [9],

$$M_3 = \left(\frac{a_1}{u_2}, \frac{a_4}{a_1}, g^{\frac{\gamma_4 - 1}{2\gamma_4}}, -\frac{\gamma_{4-1}}{2}\right)^{-1}$$

4.5

The value for the Mach number in the region 3 is effectively the exit Mach number for the effective divergent nozzle formed because of the insert. The well-known Area-Mach number relation of a nozzle can be applied to get the required area ratio,

$$\frac{A_4}{A_{4-insert}} = \left(\frac{\gamma_{4-1}}{2}\right)^{-\frac{\gamma_4+1}{2(\gamma_4-1)}} \cdot \left(\frac{\left(1+\frac{\gamma_{4-1}}{2}, M_3^2\right)^{\frac{\gamma_4+1}{2(\gamma_4-1)}}}{M_3}\right)$$

4.6

The A_{4-inser} is the area required for flow at the end of area to change due to the driver insert. This makes the flow area in remaining driver section to be A_{4-inser}. The maximum diameter of the insert can be calculated by equation 4.7,

$$D_{insert} = \sqrt{D_4^2 - \frac{4.A_{4-insert}}{\pi}}$$

where D_{insert} is the diameter of the insert and D₄ is the driver diameter.

The required diameter of the insert varies from shock to shock and does not allow for averaging out an effective area. The insert is so designed to allow for changes in the final diameter and the rate of area change to accommodate the variations in every shock.

4.3 Manufacturing of The Insert

To accommodate for variations in the specifications of the driver insert from shock to shock, the insert was designed in small sized pieces of varying diameter which can be assembled in multiple configurations. Since the Insert is mounted on the driver end-wall and acts as a cantilever, the material used for manufacture had to be light but strong. Non-corrosive properties were also required considering the type of fuels it will be directly exposed to. Aluminum Alloy 3003 was chosen since it was cost-effective for the required properties. The diaphragms used are of the same material, which ensures that the material will not absorb or react with the fuel studied.

The insert was manufactured by turning aluminum rod to the required diameters and cutting it in small pieces. Holes were drilled and tapped axially to join multiple pieces together to form the required length using grub screws as seen in the Figure 23. The details of the pieces manufactured are furnished in Table 4.

Table 4 Details of the steps of the insert.

Diameter	Length	Quantity
1/8"	1"	2
3/16"	1"	2
1/4"	1"	2
5/16"	1"	2
3/8"	1"	2
7/16"	1"	2
½″	1"	2
9/16"	1"	2
5/8"	6"	4
3/" /4	2"	3

4.7



Figure 23 Disassembled pieces of the driver insert.

Various combinations were tried experimentally over a set of pressures and temperature ranges and a configuration of the insert was found which provides acceptable results over a wide variety of temperature ranges for given pressures. A drawing of the insert is shown in Figure 24. It was also observed that the length of this configuration did not negatively affect the pressure profile for slightly higher reaction times and the area ratio did not over compensate for lower temperature shocks where the time of pressure rise is significantly lower.



All small steps are of equal lenght - 50.80 mm All dimensions are in mm

Figure 24 Configuration of the insert providing optimum performance over a wide range.

The use of the insert allows a near ideal pressure profile in the reaction region when used along with tailoring of the driver gas. The maximum effect of the driver insert is observed in a straight tube. Hong et al [12] suggests that similar technique can be used in a shock tube having a convergent area in the diaphragm region, although the area relation for a convergent shock tube is highly non-linear. The calculations to be carried out need to first account for the convergence and then calculate the required divergence in area by the driver insert to compensate for the pressure rise.

The insert was used in the shock tube having a constant bore across driver and the driven section of 1 inch. The driver has a length of 60 inches and the driven section has a length of 140 inches. The 40-inch-long insert was mounted as a cantilever from the driver end wall. The gas filling port is located approximately 7 inches away from the tip of the driver insert so that filling does not apply stress on the insert.

The pressure trace from the end wall for a shock producing 1121 K temperature at 76 atm pressure behind the reflected shock is shown in the Figure 25. The arrows mark the region over which the expected non-ideal pressure rise occurs. It can be observed from the pressure trace that the pressure is nearly constant in that region due to the use of driver insert.



Figure 25 Pressure trace from the end wall transducer for test shock at a nominal pressure of 76 atm at an ideal temperature of 1121K with non-ideal pressure rise eliminated using driver insert. The contact surface bump is evident because of untailored driver gas.

The non-ideal pressure rise becomes more prominent as the temperature in the reaction region rises. Figure 26 and

Figure 27 show the end wall pressure traces for shocks at 1207 K temperature at 37 atm and 1322 K temperature at 22 atm

respectively. The region marked by arrow shows the region over which pressure remains nearly constant as a result of compensation of non ideal pressure rise.



Figure 26 End wall pressure trace for a test shock at a nominal pressure of 37 atm and ideal temperature of 1207.67K. Non-ideal pressure rise eliminated with a tailored driver gas showing pressure in reaction region to remain constant.



Figure 27 Pressure trace from the end wall transducer for test shock at a nominal pressure of 22 atm and 1322.27K with eliminated nonideal pressure rise with a tailored driver gas to produce near constant reaction region pressure.

5 BACKFILLING OF DRIVER GAS TO EXTEND REACTION TIME

5.1 Principle

The back-filling technique utilizes the reduction in sound speeds of gases with higher molecular weights to increase the available reaction time in the shock tube without major physical or structural alterations to the shock tube. This method was suggested by Campbell et al[14]. This method increases the reaction time by delaying the arrival of the reflected driver expansion wave at the reaction region which quenches the reflected shock.



Figure 28 Schematics of driver section back filling. Driver filled with tailored primary driver gas till P4i (top). The backfill gas is filled till burst pressure (P4) is reached (bottom). Adapted from Campbell et al[14].

The change in the reaction time is the directly related to the amount of back-fill gas in the driver section. The increase in the driver length to which the back-fill gas is filled, increases the reaction time proportionally. The maximum length to which the back fill is effective depends on the rate of filling and the composition of the primary driver gas. A slow rate of filling often causes a large part of the back-fill gas to mix into the primary driver gas, which affects the driver gas tailoring and reduces the shock strength. If the fill rate is appropriate the mixing region of the back fill and primary gas will be small, thus not drastically affecting the shock formation due to the primary gas. Figure 28 shows a schematic of this technique.

5.2 Reaction Time

The reaction time is the time for which the reaction region holds the required reaction pressure and temperature conditions. The conditions in the reaction region need to be instantaneously quenched to ensure freezing of the reaction at the end of the required reaction time. Since ideally the quenching is not an instantaneous event, some chemistry is expected

to continue for a few milliseconds after beginning of the quenching. For this purpose, at UIC- High Pressure Shock Tube Laboratory the reaction time is measured from the initial pulse to the point of 80% pressure drop from the maximum value, as an empirical approximation.

Longer reaction times are required for recent projects at UIC-Shock Tube Laboratory to study the feasibility of using jet fuels for diesel applications. To test this the fuel needs to be subjected to long reaction times at low temperature (700 K – 1000 K) and high pressures (up to 300 atm). Previously the HPST was used for experiments having reaction times ranging up to 2.5 ms. To achieve the longer reactions, the operation of the shock tube was modified by applying reaction time increasing techniques suggested by Campbell et al [14] along with increasing the length of the driven section by using the driven section extensions already available at UIC – Shock Tube Laboratory.

Figure 29 shows the result of back-filling of the driver section to produce longer reaction times. The shocks depicted in the Figure 29 are generated using a well-tailored driver gas in the driver with a driver insert to produce long constant pressure environments in the reaction region. Additionally, the pressure remains completely constant for the shock at the low temperature (855 K) since the non-ideal effects are not as intense for low temperatures.



Figure 29 End-wall transducer pressure trace showing change in reaction time because of backfilling of the driver section by a low sound speed gas (Ar). The driven gas is argon and the driver gas is a tailored mix of argon in helium.

5.3 Technique

The technique of backfilling the driver with a gas having low speed of sound was primarily employed to achieve reaction times as long as 7 ms at the reaction pressure and temperature values. The driver gas responsible for formation of the shock, referred as primary driver gas in this section, is tailored to the required tailoring condition using the steps from section 3.3.2. The backfill gas is used to pressurize the driver section after the primary driver gas has been added, until the diaphragm bursts.

In UIC- Shock Tube Laboratory, the primary driver gas is helium tailored by mixing in small amounts of argon as explained in section 3.3.2. The choice of backfill gas is also argon since it has a high molecular weight resulting in a lower speed of sound. The driven gas is argon. The choice of gas is based on the availability, ease of calculation due to same specific heat ratios and cost effectiveness of the gas. Provisions were made on the UIC-HPST to connect pneumatic operating solenoid-controlled valves to carry out back filling of driver section to the burst pressure. Separate ports are available through which primary driver gas and tailoring gas can be put into the driver, before back filling. The driven section is filled in the same way as it is for conventional shocks. The steps utilized in firing the shock tube by this method are,

- 1. The driver section is filled with argon, in proportion to tailoring requirement for the intended reaction region conditions.
- 2. The driver is then filled with helium to an intermediate filling pressure (P_{4i}). This pressure gives the percentage of driver section that will be back filled since the pressure ratio of burst pressure to intermediate pressure is directly proportional to the ratio of length to which primary driver is filled over the driver length.

$$\frac{P_{4i}}{P_4} = 1 - \frac{L_{backfill}}{L_{driver}}$$

Using the above relation and knowledge of the approximate diaphragm burst pressure , one can control the length to which back fill gas should be filled assuming negligible length of the mixing region. Figure 28 gives the schematic of the back fill length.

- The driven section is now filled with the test gas to the required initial pressure (P1) needed to achieve the required reaction region conditions.
- 4. The Driver is now back-filled with the back-fill gas (Ar) till the diaphragm bursts.

5.4 Apparatus Modification

The apparatus could not be used in an as is condition to carry out the backfilling procedure. Minor modifications and new valves with gas lines were added. The back fill gas was needed to be boosted to a high pressure, like the primary driver gas. To accomplish this, one bank of high pressure cylinders was boosted to 10,000 psi with argon as the back-fill gas and the other bank was boosted to about 6,000 psi with helium and was used to make the primary driver gas.

An additional solenoid controlled, air-operated high-pressure valve was connected to the ports available on the driver end-wall as seen in Figure 30. The in-house software developed to operate the shock tube controls this valve to fire the shock tube, unlike the driver gas valve previously used. A metering valve was connected between the air-operated valve and the driver end-wall to maintain a relatively constant flow rate of the back fill. The flow rate of the metering valve was experimentally set to the most optimum value. The high-pressure cylinder bank boosted with argon was connected this valve.



Figure 30 Schematics of the shock-tube with modification to carry out back-filling of the driver section.

5.5 Discussion

The effect of back-filling the driver section with a low speed of sound gas can be observed in Figure 31 where the reaction time went up from about 3.2 ms to 5.5 ms by back-filling the driver for about half of the driver length.

The effect of back fill on the reaction time is dependent on the temperature in the reaction region but is independent of the pressure in the reaction region. As the temperature rises, for the same pressure in the reaction region, the reaction time reduces while the amount of backfill is kept nearly constant. The graph in Figure *32* depicts the change in reaction time with increase in temperature for the same amount of back fill at pressures of 20 atm and 50 atm.



Figure 31 Pressure trace from the end wall pressure transducer for test shocks having a nominal post shock pressure in the range of 25 atm showing the effect of back-filling. The driver gas mixture is tailored by mixing argon in helium. The approximated backfilled driver length is 29 inches.



Figure 32 Effect of temperature on the reaction time, with constant back-fill of driver at 50%

6 OPTIMIZED PRESSURE CHARACTERISTICS BEHIND THE REFLECTED SHOCK WAVE

The various methods to eliminate or compensate for non-ideal behavior in the shock tube when combined can allow the shock tube to perform close to the performance characteristics of the shock tube as described by the ideal shock tube theory.

The non-ideal pressure rise that occurs in the reaction region behind the reflected shock due to various effects such as boundary layers, shock attenuation and diaphragm opening behavior cannot be prevented since the exact source is not known and varies from shock to shock irrespective of reaction region conditions. The best approach to overcome this issue is to compensate for the pressure rise. Since the pressure behavior directly corresponds to the temperature behavior, this compensation will also maintain the temperature near constant when the pressure is maintained to a constant value. The use of driver inserts with varying cross section area, as described previously allows for this compensation.

The contact surface interaction of the shock in a single pulse shock tube is an unwanted phenomenon and often causes a drastic sudden pressure rise. This interaction can be prevented by the tailoring of the driver gas so that the impedance conditions as given in equation 3.1 across the contact surface can be maintained, as suggested by the ideal shock tube theory. When this condition is maintained the contact surface does not act as obstacle for the reflected shock and allows it to freely a pass through it while the contact surface remains stationary.

When the driver insert is used, and the shock is fired using a tailored driver gas, a well behaving pressure characteristic can be observed behind the reflected shock. This pressure characteristic provides a close to ideal environment to carry out chemical kinetic study of fuels. The reaction time also increases slightly for a tailored driver gas as seen in Figure 33. This occurs due to the reduced speed of sound in the driver section because of mixing of argon in primary driver gas (helium).

The comparison of shock profiles in Figure 33, Figure 34, Figure 35 and Figure 36 between optimized and regular shock shows that the effect of non-ideal effects increases with increases in temperature. High temperature reaction regions are more difficult to optimize when compared to low temperature reaction regions due to the greater extent of non-ideal pressure rise over time which may occur due to a delay in shock formation. This can be seen in Figure 33 and Figure 34. The higher temperature reaction region generates shocks that have higher speeds which may lead to complete shock formation further downstream in the driven section, adding to viscous effects at the boundary layer which is evident in Figure 33.

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Figure 33 End-wall pressure transducer pressure traces for two shocks, regular and optimized giving similar reaction region conditions. Reaction region has nominal pressure of 40 atm and ideal temperature of about 1350K.



Figure 34 End-wall pressure transducer pressure traces for two shocks, regular and optimized giving similar reaction region conditions. Reaction region has nominal pressure of about 39 atm and ideal temperature range of 1150K

It is also observed that the lower temperature shocks are relatively well behaved, even in the absence of optimization

techniques as can be seen in the Figure 35. For shocks up to 1100 K a completely ideal profile can be obtained by employing

the methods described in this thesis. The non-ideal pressure rise for reaction region temperatures up to 1100 K is relatively

low and easier to compensate for as seen in Figure 35. At temperatures below 1100 K, the effect of contact surface interaction



with the shock does not cause as adverse an effect as it does for higher temperatures.

Figure 35 End-wall pressure transducer pressure traces for two shocks, regular and optimized giving similar reaction region conditions. Reaction region has nominal pressure of about 30 atm and ideal temperature range of 850 K

The Figure 36 shows the comparison of two shock profiles having approximately the same initial reaction region pressure. It can be seen in Figure 36 that the regular shock profile undergoes a significant rise in pressure whereas the pressure remains nearly constant when driver gas is tailored to optimize the shock. The reaction time is measured at 80% pressure of the maximum pressure. The calibrated temperature for the regular shock will be higher than that for the optimized shock since the average pressure in the reaction region over the reaction time is higher in the regular shock. The reaction time for optimized shock profile based on the 80% pressure value is higher due to a slower rate of pressure drop as evident in Figure 36.

After application of the optimizing techniques to the shock tube, we can achieve higher reaction times than that for regular shocks since the 80% pressure from max pressure is much lower leading to a longer reaction time. The reaction times, although increased, are not sufficient to carry out analysis of fuels at lower temperatures as needed by the current projects at the lab. The optimization techniques are then combined with the technique of driver backfilling with a low speed of sound gas as described in chapter 5.



Figure 36 End-wall pressure transducer pressure traces for two shocks, regular and optimized having approximately same initial reaction region pressure. Reaction region has ideal temperature range of 1050 K.



Figure 37 Pressure traces from end wall transducer for shocks with various amounts of back-fill.

With the use of driver backfilling, reaction times as high as 8 ms are obtained, as seen in Figure 37. This increase in reaction time is achieved with no modification of the physical characteristics of the shock tube. The addition of ancillary techniques alone has allowed increase of the reaction time by as much as 4 times by using this technique.

In the comparison shown in Figure 37 a reaction time of 3.26 ms was obtained for a shock producing 25 atm and 817 K without any backfill. When the tube was backfilled to about 50% of the driver length a reaction time of 5.46 ms was observed at 20 atm and 795 K. The tube when back-filled to 75% of the driver length obtained a reaction time of 7.51 ms at 20 atm and 805 K. This shows that for every 25% of back-fill in the driver section, the reaction time can be increased by about 2 ms. There was negligible effect of backfilling the driver section below 50% since the primary driver already has a high amount of argon mixed in it for driver gas tailoring.

7 TEMPERATURE CALIBRATION USING THE OPTIMIZED REACTION REGION CHARACTERISTICS

The temperature plays a significant role in analysis of chemical kinetics of hydro-carbon fuels. The accuracy of temperature measurement in the reaction region of the shock tube directly affects the accuracy of the analytical results obtained for the shocked test gas. The temperature can be estimated using ideal gas relations as suggested in the ideal shock tube theory but due to non-idealities in the shock tube as explained in section 4.1 the ideal equations cannot accurately yield temperatures in the reaction region.

The temperature rise in the shock tube takes place on the order of milliseconds. To measure this instantaneous change in temperature conventional temperature sensors such as thermocouples or thermistors cannot be used as the time required by them for temperature detection is high. The change in flow velocities near the end-wall may also affect performance of these sensors. Optical methods such as laser spectroscopy are commonly used to measure temperatures in such situations. These provide highly accurate measurements but have constraints on the type of gas that needs to be used in the shock tube. The optical properties such as emissivity, absorptivity ,electronic excitation etc needs to be considered in choosing the gas. The high pressures that the UIC-HPST develops makes it difficult to add provisions such as windows needed carry out optical measurements. These constraints lead to the use of external chemical thermometers to evaluate the temperature in the reaction region of UIC-HPST.

7.1 <u>Temperature Measurement by Chemical Methods</u>

The use of chemical methods to measure temperature in the high-pressure shock tube allows a means for measurement of the temperature in the region since they are capable of accounting for the thermodynamics and gas dynamics of the end gas. It provides a practical estimate of the temperature in the reaction region.

The chemical thermometer is a chemical species whose unimolecular rate constant for dissociation is well known and defined. The chemical thermometers are shocked in the shock tube like the fuel to be tested would be and the extent to which it dissociates is measured. The unshocked sample is used as reference for the initial amount of chemical thermometer present in the calibration mixture. The mixture is then shocked in the shock tube by shocks which produce varying temperatures, as estimated by ideal shock tube theory for a pre-defined reaction time. A sample after each shock is analyzed using a GC. The shock velocity is directly measured by the pressure transducers on the side walls of the shock tube. The extent of reaction can be known by subtracting the amount of chemical thermometer found in the shocked sample from the unshocked sample.

When the extent of reaction is known, the average temperature can be calculate using the known rate constants and activation energy for the chemical thermometer by,[15]

$$T_i = \frac{\left(\frac{-E}{R}\right)}{\ln\left\{\left[\frac{\ln(1-x)}{A \cdot t}\right]\right\}}$$

where, E is the activation energy, R is the universal gas constant, A is the pre-exponential factor, t is the reaction time and x is the extent of reaction,[15]

$$x = \frac{CT_0 - CT_i}{CT_0}$$

where CT_0 is the amount of chemical thermometer in the unshocked sample and CT_i is the amount post shock.

The average temperatures derived from equation 7.1 can be plotted against the shock velocity measured by the transducers to form the temperature calibration curve. The equation of the curve can be used to approximate the temperature for a given velocity. When fuel is shocked for analysis, the temperature of the reaction region can be predicted from the calibration curve using the measured shock velocity.

7.2 Chemical Thermometers

The chemical thermometers need to have a well-defined unimolecular decomposition rate with just one reaction pathway. This allows the use of just one reaction rate constant for calculation using equation 7.1 throughout the range of shock speeds. The chemical thermometer should have a well-established and validated decomposition rate expressions to avoid any systematic errors and uncertainties in the kinetic measurements. A wide range of decomposition temperatures is preferred for the chemical thermometer so that a single thermometer can cover a wide range of calibration, but often most chemical thermometers have a range of not more than 200 K, which leads to use of two or more chemical thermometers to calibrate over a wider temperature range. The two chemical thermometers used are 1,1,1 – trifluoroethane and cyclopropanecarbonnitrile.

7.2.1 <u>1,1,1-TRIFLUOROETHANE – TFE</u>

One of the most commonly used chemical thermometer is 1,1,1, - trifluoroethane since it has very well-known rate constant parameters and has a decomposition range from 1200 K to 1350 K which is the most common range for chemical kinetic experiments of hydrocarbons. TFE does not react significantly at temperatures below 1200 K making it impossible to evaluate

7.2

7.1

lower temperatures. Similarly, for temperatures above 1350 K since the parent TFE molecule breaks down too fast giving a very high extent of reaction. The unimolecular decomposition occurs as

$$CH_3CF_3 \rightarrow CH_2CF_2 + HF$$

As suggested by Matsugi et al[16] the value of high pressure rate coefficient parameters used for calculating the temperature based on the unimolecular decomposition are,

$$A = 3.33 \times 10^{14}$$

 $-E/R = 37363$

7.2.2 CYCLOPROPANECARBONITRILE - CPCN

The required range of temperatures for chemical kinetic analysis for hydrocarbon jet fuels goes as low as 900 K. To calibrate temperature for the lower temperatures CPCN is used since it has a decomposition range of 900 K to 1100 K beyond which the extent of reaction is in the top 90% range or below the 10% range, having virtually no effect on the calibrated temperature. However when the calibrations from CPCN and TFE are combined a complete range from 900 k to 1400 k can be obtained which is sufficient to study the chemical kinetics of hydrocarbon fuels in pyrolysis and oxidation.

The rate constants for this chemical thermometer were calculated by Lifshitz et al [17] based on unimolecular isomerization of cyclopropanecarbonitrile. The isomerization leads to formation of cis and trans crotonitrile($CH_3CH = CHCN$) and vinylacetonitrile ($CH_2 = CHCH_2CN$).

$$A = 3.2 \times 10^{14}$$

 $-E/R = 29106.223$

7.3 Temperature Calibration

Temperature calibrations were carried out for the UIC-HPST for the optimized shocks. The most optimum configuration of the shock tube which gave ideal like post shock conditions was used to shock heat the chemical thermometers. The expected reaction time is in the range of 3 ms to 4 ms, at which time the pressure drops to 80% of the maximum pressure. The chemical thermometers were diluted in an argon bath to values of about 200ppm. This test gas was then shocked in the shock tube.

The test gas was analyzed in one of the 7890B GC connected to the HPST to calculate the initial amount of chemical thermometer present in the test gas. The post shock test samples were analyzed to measure the extent to which the chemical

thermometer underwent unimolecular decomposition at each shock velocity. The temperature for each shock velocity can be calculated using the equation 1.6.

The calibrated temperatures obtained using the thermometer rate parameters can be compared with the ideal temperatures calculated using the ideal shock tube theory for the known velocities of every shock. This comparison in Figure 38 and Figure 39 shows the difference of the ideal temperature from the actual temperature because of non-idealities.

The shock tube was set to a constant diameter using the driver area reduction insert. The area reducing driver insert was used to compensate for the non-ideal effects in the reaction region. The driver gas was tailored for every shock to avoid the occurrence of the contact surface bump. The driver was not back filled since the calibration was done for regular reaction times. The length of driver section was kept at 60 inches and driven section was 140 inches long.

7.4 Result of Temperature Calibration

The first set of calibration experiments were carried out using TFE at a nominal pressure of 25 atm. The TFE calibration curve spreads over a 200 K temperature range from 1200 K to 1350 K as shown in Figure 38.



Figure 38 Calibration Curve for TFE at 25 atm, from 1200 K to 1350 K.

The calibration results as seen in Figure 38 show that most of the calibrated temperatures are close to their respective ideal temperatures. Several points can be seen away from the ideal temperature because of uncertainties in the

measurements due to greater difficulty in optimizing high temperature shocks. While most experiments were achieved with optimized shock profiles, optimization of some shocks was not successful.

The second set of calibrations were carried out using CPCN to cover the range of temperatures from 900 k to 1100 K at 25 atm as shown in Figure 39.



Figure 39 Calibration Curve for CPCN at 25 atm, from 900 K to 1100 K.

The calibration results using CPCN as the chemical thermometer shown in Figure 39 match the ideal temperatures more closely when compared to TFE since maintaining an optimized profile for shocks in the temperature range for CPCN is easier and more successful. Scatter is still occurring in the calibration since CPCN is much heavier making its detection in gas chromatography difficult.



Figure 40 Temperature Calibration at 25 atm with two chemical thermometers , CPCN and TFE.



Figure 41 Overall temperature calibration curve for temperature ranging from 900 K - 1350 K at 25 atm.

The calibration data are individually plotted with the temperature calculated using the shock relations and ideal shock tube theory as illustrated by Figure 40. The calibration lines for both the thermometers have very similar slopes and are inclined in the same direction. The overall calibration curve was obtained for a temperature range of 900 K to 1350 K at 25 atm by combining the individual calibration curves to form a single curve as seen in Figure 41. This curve can be directly used to approximate the temperature in the reaction region over the complete range for the measured shock velocity. The high agreement observed in the overall temperature calibration curve shows that the optimized shock develops conditions very close to conditions as calculated by the ideal shock tube theory[1].

The agreement of the calibrated temperature with the temperature calculated by ideal shock tube relations when the reaction region pressure is nearly constant justifies the use of chemical thermometer in shock tube studies to estimate the temperature in the reaction region. This further implies that calibrated temperatures achieved in the shock tube for shocks closely approximates the average temperature of the reaction region based on the pressure characteristic of that shock. In the case of non-optimized shocks, the temperature calibration may not be in agreement with the ideal temperatures but the calibrated temperature accounts for the non-ideal effects to provide an accurate estimation of the average temperature.

8 CONCLUSION

The techniques discussed in chapter 1 and 3 for optimization of the pressure and temperature characteristics in a single pulse high pressure shock tube have been found effective in developing constant pressures and temperatures in the reaction region for the required time. The temperatures obtained in the reaction region are in agreement with the temperatures calculated based on incident shock Mach number using the ideal shock tube theory as depicted by the overall temperature calibration curve in Figure 41. This also justifies the use of chemical thermometers for measurement of temperatures in the post shock region of the shock tube.

The reaction time can be significantly increased without physical modifications to the shock tube by using driver gas back-filling as explained in the Chapter 5. Reaction times were increased by as much as 4 times of those observed without employing the technique. The reaction time can be further increased by carrying out more modifications to allow for back filling of the gas when the shock tube has a constant driver and driven diameter. New ports need to be machined on the driver diameter reducing insert to allow the backfilling ports to fill gas into the bore of the insert. A further increase in reaction time is expected by employing the backfilling technique in the presence of a driver insert and by a tailored primary driver gas for the shock tube having a constant bore of 1 inch.

The temperature calibrations should be carried out at various pressures with the optimized profile to verify that the agreement between the ideal values and calibrated values exist with no pressure dependency. The temperature calibrations are highly affected by the reaction times since it directly factors into the equation to compute the calibrated temperature based on extent of reaction. Thus calibrations need to be carried for various reaction times before fuels are studied at those reaction times.

Finally, all the techniques will be applied in combination to carry out the analysis of low cetane number fuels at low temperatures and high pressures. The longer reaction times which are needed to allow for the reactions to occur at low temperatures for these fuels can be achieved.

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APPENDIX A



Figure 42 Schematics of the UIC-HPST Facility

APPENDIX B

T1 =	373									
Г5 =	1400		a1=	359.7065	a3 =	472.5296	M3 =	0.927077	P3 =	265.1543612
5/T1 =	3.753351206		MW1 =	39.948						
∕ls =	2.1		a4 =	618.5533						
									A4/A1=	4
1 =	50.38562684		T4 =	373					MW4-1 =	<u>39.948</u>
25 =	1000.00	68.02721	R4 =	615.4556					MW4-2 =	4.004
4 =	1019.152918		P4 =	1019.153					P4-1 =	269.5163727
2=	265.1543612		MW4=	13.50944	P4-Ar	269.5164			P4-2 =	749.636545
12 =	438.0711337				P4-He	749.6365			%4-1 =	0.264451358
13 =	438.0711337								%4-2 =	0.735548642
13a =	0								Total % =	1
									Avg MW4 =	13.5094396
P5/P2 = 3.77138809								γ1 =	1.67	
								γ4 =	1.67	
									α1	4
									α4	4
									(γ1+1)/(γ1-1)	4
									(γ4+1)/(γ4-1)	4
									(γ1+1)	2.666666667
									(γ4+1)	2.666666667
									(γ1-1)	0.666666667
									(γ4-1)	0.666666667
									(2*γ1)	3.333333333
									(2*γ4)	3.333333333
									(3γ1-1)	4
									(3γ4-1)	4
									R Constant =	8314.4598

Microsoft Excel Sheet to Calculate Driver Gas Tailoring for a constant bore shock tube.

The cells with yellow color are required input values. The unit for pressures in the sheet is psi and for temperatures is Kelvin. The solution is calculated using a background

sheet, acting as iterator. The spreadsheet with instructions is available in the supplemental materials under the name *Driver Gas Tailoring Conventional Tube.xls.*
Microsoft Excel Sheet to Calculate Driver Gas Tailoring for a convergent shock tube	Microsoft Excel S	Sheet to Calculate	e Driver Gas T	Tailoring for a	convergent shock tube
---	-------------------	--------------------	----------------	-----------------	-----------------------

T1 =	373									
T5 =	1400	a1 =	= 359	9.7065	a3 =	472.5296	M3 =	0.927077	P3 =	265.1543612
T5/T1 =	3.753351206	MM	V1= 3	39.948	a3a=	561.0578	M3a =	0.219	P3a =	625.7365924
					a3b =	489.7588			P3b=	317.1502724
Ms =	2.1	a4 =	= 60	02.015						
					P4/P3a	1.422324			A4/A1 =	4
P1=	50.38562684	T4 =	=	373	P3a/P3b	1.972997			MW4-1 =	<u>39.948</u>
P5 =	1.00E+03	68.02721 R4 =	= 582	2.9845	P3b/P3	1.196097			MW4-2 =	4.004
		P4 =	= 890	0.0003					P4-1 =	253.9929683
P2=	265.1543612	MM	N4= 14.3	26189	P4-Ar	253.993			P4-2 =	636.0073514
u2 =	438.0711337				P4-He	636.0074			%4-1 =	0.285385255
u3 =	438.0711337								%4-2 =	0.714614745
u3a =	122.8716521								Total % =	1
									Avg MW4 =	14.26188761
P5/P2 =	3.77138809								γ1=	1.67
									γ4 =	1.67
									α1	4
									α4	4
									(y1+1)/(y1-1)	4
									(γ4+1)/(γ4-1)	4
									(γ1+1)	2.666666667
									(γ4+1)	2.666666667
									(γ1-1)	0.666666667
									(γ4-1)	0.666666667
									(2*γ1)	3.333333333
									(2*γ4)	3.333333333
									(3γ1-1)	4
									(3γ4-1)	4
									R Constant =	8314.4598

The cells with yellow color are required input values. The cell marked in orange is an assumed value used as input. The unit for pressures in the sheet is psi and for temperatures is Kelvin. The solution is calculated using a background sheet, acting as iterator. The spreadsheet with instructions is available in the supplemental materials under the name *Driver Gas Tailoring Convergent Tube.xls.*

APPENDIX C

Microsoft Excel Sheet used to calculate the specifications of the driver insert

			Calculation of sh	ock Tube	Parameters by	Normal	Shock T	ube The	ory for a	Convent	tional Sho	ock Tube							
D1 -	0	0.0000E±00	P4 -		#DIV/01	D3 -	#DIV/01		D2-	#DIV/01		D5 -	#DIV/01			\A/c -		n	
T1 =			T4 =		#DIV/0!	T3 =	#DIV/0		T2=	#DIV/0		T5=	#DIV/0!			Ms =	#DIV/0		
v1 =	0.00		v4 =	0.00	n	10						1.5				Wr =	#DIV/0		
R1 =	208.1320667	,	R14=	#DIV/0!	<u>-</u>	M3 =	#DIV/0!									un =	#DIV/0!		
MW1 =	39.948	1	MW4 =	#DIV/0!		u3 =	#DIV/0!	•	u2 =	#DIV/0!		P5max		0 T5 =	C				
a1 =	0)	a4 =	#DIV/0!		a3 =	#DIV/0!		a2=	#DIV/0!		P5start		0					
ρ1=	#DIV/0!		ρ4 =	#DIV/0!															
P2/P1 =	#DIV/0!		P3/P4 =	#DIV/0!		P4/P5 =	#DIV/0!					P5/P1 =	#DIV/0!					MW4-1 =	39.948
T2/T1 =	#DIV/0!		T3/T4 =	#DIV/0!	•							P5/P2 =	#DIV/0!					MW4-2 =	4.004
P4/P1 =	#DIV/0!											T5/T1 =	#DIV/0!					P4-1 =	150
					Impedence	#DIV/0!	1					T5/T2 =	#DIV/0!					P4-2 =	-150
																		%4-1 =	#DIV/0!
tpeak =	0.846	i																%4-2 =	#DIV/0!
													Total Insert Length =	-0.52				Total % =	#DIV/0!
P4 for P5max	#DIV/0!		P4s/P4m =	#DIV/0!		M6 =	#DIV/0!		A4 =	#DIV/0!	Dinsert =	#DIV/0!	Lstart =	0.52				Avg MW4 =	#DIV/0!
P4 for P5start	#DIV/0!		a4'/a4 =	#DIV/0!		A1/A4 =	#DIV/0!		A1 =	C) Ainsert =	#DIV/0!	Lend =	0.8805652					
													Area Change Length	= 0.3605652				α1	-1
							R. A. A	pher &	D. R. Wh	ite								α4	-1
											Instructio	ns				1		(γ1+1)/(γ1-1)	-1
Driven Length =	0)	Driver Diameter =	(Area Driver (A4) =	0.00)	Zc	#N/A		1. Input th	he obsered	and initial conditions	of the shock tu	be in the			(y4+1)/(y4-1)	-1
Driver Length =	Ő		Driven Diameter =	(Area Driven (A1) =	= C)	Zs	#DIV/0!		yellow and orange cells. 2. Enter the location of tip of the insert found by using x-t diagrams (refer to thesis) in cell 018. 3. Obtain the relation between reaction time and lenght of the driver					(γ1+1)	1		
Total Length =	0)	A4/A1=	#DIV/0!	A1/A4 =	#DIV/0!		Gm =	#DIV/0!							(γ4+1)	1		
																(γ1-1)	-1		
M3 =	#DIV/0!	P3 =	#DIV/0!	a3 =	#DIV/0!			A4/A1 =	#N/A							(γ4-1)	-1		
M3a =	#N/A	P3a =	#N/A	a3a =							aroa chan	lagrams (re	eter to thesis). Using tr	is equation of	tain end of			(2*γ1)	0
M3b =	#DIV/0!	P3b =	#DIV/0!	a3b =	#DIV/0!						4 Areach	nange requi	ired can be obtained fr	om H19 18 a	nd I19			(2*γ4)	0
M3b' =	#DIV/0!	P3b' =	#DIV/0!	a3b'=	#DIV/0!						5. The res	sultinterac	tion of the shock and d	iscontinuity ca	n be seen			(3γ1-1)	-1
											in cell G14	4. If value i	s greater than 1 then it	reflects as an o	expansion			(3γ4-1)	-1
											wave but	if it is less	than 1 ,shock will refle	ct from the dis	continuity.			R Constant =	8314.4598
																		Readouts	Inputs / Readouts
University of	of Illinois a	at Chicag	o - High Press	ure Sho	ck Tube Lab	orator	у											Variation (Formula)	Ideal/Calculated
Jai M. Mehta Pr	of. Kenneth Bre	ezinsky - Depo	artment of Mechanico	al & Industri	al Engineering													Linked Value	Not needed

The sheet above uses the yellow cells as input. The orange cells show readouts to verify the calculations and green cells show values linked from other back

ground sheets. The sheet shown above is the primary sheet which uses two more background sheets act as iterator. The spreadsheet with instructions is available in the

supplemental materials under the name *Driver Insert Design.xls.*

APPENDIX D

Setpoint

(Initial)

Injection Source and Location									
Injection Source: GC Valve									
Injection Location: Both									
======================================									
GC									
GC Summary									
Run Time	37.333 min								
Post Run Time	0 min								
Oven									
Equilibration Time	0.5 min								
Max Temperature	300 °C								
Maximum Temperature Override	Disabled								
Slow Fan	Disabled								
Temperature									
Setpoint	On								
(Initial)	45 °C								
Hold Time	5 min								
Post Run	260 °C								
Program									
#1 Rate	5 °C/min								
#1 Value	80 °C								
#1 Hold Time	3 min								
#2 Rate	15 °C/min								
#2 Value	150 °C								
#2 Hold Time	3 min								
#3 Rate	15 °C/min								
#3 Value	250 °C								
#3 Hold Time	8 min								

375 °C

Off

Post Run

Column#1

Column Outlet Pressure

Column #1

Column Information Temperature Range Dimensions Column lock In Out (Initial) Pressure Flow Average Velocity Holdup Time Pressure Setpoint (Initial) Post Run

Column #2

Column Information Temperature Range Dimensions Column lock In Out (Initial) Pressure Flow Average Velocity Holdup Time Pressure Setpoint (Initial) Post Run

Front Detector TCD

Makeup Heater Reference Flow Makeup Flow Filament

0°C

0 psi

J&W 113-4362 GS-GasPro -60 °C—260 °C (325 °C) 60 m x 320 μm x 0 μm Unlocked Aux EPC 1 He Back Detector FID 45 °C 15.885 psi 2 mL/min 27.579 cm/sec 3.626 min

On 15.885 psi 10 psi

J&W 19095P-MS0E HP-MOLSIV Megabore -60 °C—300 °C (325 °C) 30 m x 530 μm x 50 μm Unlocked Aux EPC 2 ArMe Front Detector TCD 45 °C 10 psi 6.7956 mL/min 60.791 cm/sec 0.82249 min

Off 10 psi 10 psi

Excluded from Affecting GC's Readiness State
He
On 100 °C
Off
Off
Off

Negative Polarity

Off

Back Detector FID						
Makeup	Не					
Heater	On 320 °C					
H2 Flow	On 40 mL/min					
Air Flow	On 450 mL/min					
Makeup Flow	On 30 mL/min					
Carrier Gas Flow Correction	Does not affect Makeup or Fuel Flow					
Flame	On					
Valve 1						
Туре	Gas Sampling Valve					
GSV Loop Volume	0.25 mL					
Load Time	0.01 min					
Inject Time	5 min					
Valve 2						
Туре	Gas Sampling Valve					
GSV Loop Volume	1 mL					
Load Time	0.01 min					
Inject Time	5 min					
Aux EPC 1,2,3						
Aux EPC 1 He						
Aux EPC 1 He	Supplies Column 1					
Aux EPC 2 ArMe						
Aux EPC 2 ArMe	Supplies Column 2					
Aux EPC 3 N2						
	Excluded from Affecting GC's Readiness State					
Pressure						
Setpoint	Off					
(Initial)	10 psi					
Post Run	0 psi					
Valve Box						
Heater	On 150 °C					
Signals						
Signal #1: Front Signal						
Description	Front Signal					
Details	Front Signal (TCD)					
Save	Off					
	64					

Data Rate

200 Hz

Signal #2: Back Signal	
Description	Back Signal
Details	Back Signal (FID)
Save	On
Data Rate	20 Hz
Run Time Events	
Run Time Events	
#1 Time	0.001 min
#1 Event	Valve
#1 Position	Valve 1
#1 Setpoint	On
#2 Time	0.001 min
#2 Event	Valve
#2 Position	Valve 1
#2 Setpoint	On
CPCN_GasPro.m	
Injection Source and Location	
Injection Source: GC Valve	
Injection Location: Both	

Agilent 7890B

GC

GC Summary	
Run Time	34.5 min
Post Run Time	0 min
Oven	
Equilibration Time	0.5 min
Max Temperature	300 °C
Maximum Temperature Override	Disabled
Slow Fan	Disabled
Temperature	
Setpoint	On
(Initial)	40 °C

Hold Time	1 min
Post Run	250 °C
Program	
#1 Rate	20 °C/min
#1 Value	150 °C
#1 Hold Time	3 min
#2 Rate	20 °C/min
#2 Value	250 °C
#2 Hold Time	20 min
Thermal Aux 1 (Nickel Catalyst)	
Temperature	
Setpoint	Off
(Initial)	375 °C
Post Run	0°C
Column	
Column Outlet Pressure	0 psi
Column #1	
Column Information	J&W 113-4362 GS-GasPro
Temperature Range	-60 °C—260 °C (325 °C)
Dimensions	60 m x 320 μm x 0 μm
Column lock	Unlocked
In	Aux EPC 1 He
Out	Back Detector FID
(Initial)	40 °C
Pressure	19.306 psi
Flow	2.6849 mL/min
Average Velocity	33.516 cm/sec
Holdup Time	2.9837 min
Pressure	
Setpoint	On
(Initial)	19.306 psi
Post Run	10 psi
Column #2	
Column Information	J&W 19095P-MS0E HP-MOLSIV Megabore
HP-MOLSIV Megabore	
Temperature Range	-60 °C—300 °C (325 °C)
Dimensions	30 m x 530 μm x 50 μm
Column lock	Unlocked
In	Aux EPC 2 ArMe
Out	Front Detector TCD
(Initial)	40 °C
	66

Pressure	3.4316 psi
Flow	2 mL/min
Average Velocity	21.51 cm/sec
Holdup Time	2.3245 min
Pressure	
Setpoint	On
(Initial)	3.4316 psi
Post Run	10 psi
Front Detector TCD	***Excluded from Affecting GC's Readiness
	State***
Makeup	He
Heater	On 100 °C
Reference Flow	Off
Makeup Flow	Off
Filament	Off
Negative Polarity	Off
Back Detector FID	
Макеир	He
Heater	
H2 Flow	
Air Flow	On 450 mL/min
Carrier Gas Flow Correction	Does not affect Makeup or Fuel Flow
Flame	On
Valve 1	
Туре	Gas Sampling Valve
GSV Loop Volume	0.25 mL
Load Time	0.01 min
Inject Time	5 min
Valve 2	
Туре	Gas Sampling Valve
GSV Loop Volume	1 mL
Load Time	0.01 min
Inject Time	5 min
AUX EPC 1 Has	
	Supplies Column 1
Aux EPC 2 ArMe	
Aux EPC 2 ArMe	Supplies Column 2
	67

Aux EPC 3 N2

	Excluded from Affecting GC's Readiness State
Pressure	
Setpoint	Off
(Initial)	10 psi
Post Run	0 psi
Valve Box	
Heater	On 150 °C
Signals	
Signal #1: Front Signal	
Description	Front Signal
Details	Front Signal (TCD)
Save	Off
Data Rate	200 Hz
Signal #2: Back Signal	
Description	Back Signal
Details	Back Signal (FID)
Save	On
Data Rate	20 Hz
Run Time Events	0.001 min
#1 liffe	
#1 Event	
#1 Setpoint	On .
#2 Time	0.001 min
#2 Event	Valve
#2 Position	Valve 1
#2 Setpoint	On

APPENDIX E

CPCN Calibration

Date	Feb-18			
Nominal Pressure	25	atm	А	3.20E+14
Temperature Range	900-1150	К	E/R	-29106.23

CPCN in Mixture (FID counts) 71.91868262

Shock No.	File Name	Velocity	CPCN Remaining (FID counts)	Ideal Temperature	Reaction Time	х	ln(1-X)	A*t	(-ln(1- X)/A*t)	Calibrated temperature
14	02062018_CPCN_01	638.6321264	47.93019099	1035.238247	0.0042	0.3336	-0.4058	1.342E+12	3.023E-13	1009.671942
15	02062018_CPCN_02	623.1926539	53.78781812	991.7640969	0.0043	0.2521	-0.2905	1.373E+12	2.115E-13	997.3212384
16	02062018_CPCN_03	640.0201277	25.25536171	1039.191653	0.0038	0.6488	-1.0465	1.226E+12	8.537E-13	1047.395821
17	02062018_CPCN_04	649.1006856	25.43709294	1065.240246	0.0037	0.6463	-1.0393	1.186E+12	8.766E-13	1048.392894
18	02062018_CPCN_05	647.1639939	28.57428544	1059.657698	0.0039	0.6027	-0.9230	1.24E+12	7.442E-13	1042.244756
19	02062018_CPCN_06	604.2781917	66.63269778	939.7482207	0.0037	0.0735	-0.0763	1.198E+12	6.373E-14	957.9404898
20	02072018_CPCN_01	646.2471395	14.57658577	1057.019949	0.0036	0.7973	-1.5961	1.144E+12	1.395E-12	1066.241642
21	02072018_CPCN_02	669.2318674	3.277663984	1124.138841	0.0037	0.9544	-3.0884	1.171E+12	2.638E-12	1091.712206
23	02072018_CPCN_04	634.3331409	47.60190008	1023.040901	0.0040	0.3381	-0.4127	1.264E+12	3.264E-13	1012.370993

CPCN Calibration Shocks

Nominal Pressure	25 atm	Diaphragms	Brass	0.020" / 0.013"
Shock Tube Temperature	373 К	Driver Length		60 "
Primary Driver Gas	He + Ar	Insert Length		50"
Primary Driven Gas	Ar + CPCN	Driver Diameter		1"

[Next Day]

Shock No.	Date	File name	Reaction Time - 80% [s]	P5 - Max [psi]	P5-80% [psi]	P5 - Max [atm]	Tailoring Gas -Ar [psi]	Driver pressure - P4 [psi]	Driven Pressure - P1 [psi]	Velocity [ms-1]	Ideal Temperature - T5 [K]
11	5-Feb-18	02052018_CPCN_02	0.00417	409.70	295.04	27.87	180	620	40.9	643.63	1049.52
15	6-Feb-18	02062018_CPCN_02	0.00429	307.10	223.04	20.89	180	460	28.3	623.19	991.76
16		02062018_CPCN_03	0.00383	338.10	249.92	23.00	180	480	25.7	640.02	1039.19
17		02062018_CPCN_04	0.00371	368.90	272.00	25.10	175	505	28.9	649.10	1065.24
18		02062018_CPCN_05	0.00388	325.60	240.00	22.15	170	480	25.6	647.16	1059.66
19		02062018_CPCN_06	0.00374	361.70	256.00	24.61	180	480	41.7	604.28	939.75
20	7-Feb-18	02072018_CPCN_01	0.00357	342.00	254.08	23.27	170	505	24.4	646.25	1057.02
21		02072018_CPCN_02	0.00366	333.00	249.92	22.65	165	480	20.6	669.23	1124.14
23		02072018_CPCN_04	0.00395	321.10	234.32	21.84	170	480	28.2	634.33	1023.04

Mixture Details

	Pvac	0.0396	Torr
+	\mathbf{P}_{fuel}	5.53	Torr
+	\mathbf{P}_{Ne}	22.15	Torr
+	\mathbf{P}_{Ar}	34.91	atm
	Ptotal	33.47	atm

Concentration

220.28 ppm

TFE Calibration

Date	Dec-17			
Nominal Pressure	25	atm	А	3.33E+14
Temperature Range	1200-1350	К	E/R	-37363

CPCN in Mixture (FID counts) 36.62190079

Shock No.	File Name	Velocity	TFE Remaining (FID counts)	Ideal Temperature	Reaction Time [s]	х	ln(1-X)	A*t	(-ln(1- X)/A*t)	Calibrated temperature
4	12142017_TFE_01	709.19	33.3651	1245.79	0.00294	0.0889	-0.0931	9.791E+11	9.512E-14	1246.11
7	12142017_TFE_04	691.83	34.4622	1192.18	0.00310	0.0590	-0.0608	1.031E+12	5.897E-14	1226.55
10	12152017_TFE_02	709.95	32.8517	1248.18	0.00340	0.1030	-0.1086	1.133E+12	9.588E-14	1246.44
11	12152017_TFE_03	728.08	25.2659	1305.54	0.00323	0.3101	-0.3712	1.077E+12	3.447E-13	1302.02
13	12152017_TFE_05	715.45	33.0939	1265.44	0.00317	0.0963	-0.1013	1.057E+12	9.584E-14	1246.43
14	12152017_TFE_06	749.36	21.1424	1374.60	0.00330	0.4227	-0.5494	1.097E+12	5.006E-13	1319.18
15	12182017_TFE_01	698.55	34.5959	1212.80	0.00326	0.0553	-0.0569	1.086E+12	5.243E-14	1221.84
16	12182017_TFE_02	740.01	23.7800	1344.02	0.00330	0.3507	-0.4318	1.1E+12	3.927E-13	1307.97
18	12182017_TFE_04	764.44	12.8481	1424.63	0.00309	0.6492	-1.0474	1.03E+12	1.017E-12	1353.02
20	12182017_TFE_06	747.69	21.0029	1369.11	0.00343	0.4265	-0.5560	1.142E+12	4.869E-13	1317.89
21	12192017_TFE_01	763.27	12.6415	1420.71	0.00297	0.6548	-1.0637	9.874E+11	1.077E-12	1355.86
24	12192017_TFE_04	747.53	15.6569	1368.57	0.00318	0.5725	-0.8497	1.06E+12	8.018E-13	1341.49
28	12202017_TFE_02	682.69	34.4311	1164.39	0.00374	0.0598	-0.0617	1.246E+12	4.952E-14	1219.56
29	12202017_TFE_03	717.11	32.0586	1270.69	0.00351	0.1246	-0.1331	1.169E+12	1.139E-13	1253.63
31	12202017_TFE_05	741.00	18.0068	1347.23	0.00339	0.5083	-0.7099	1.128E+12	6.294E-13	1329.93
32	01182018_TFE_01	737.79	20.4911	1336.81	0.00309	0.4405	-0.5807	1.03E+12	5.64E-13	1324.75

TFE Calibration Shocks

Nominal Pressure	25 atm	Diaphragms	Brass	0.020" / 0.013"
Shock Tube Temperature	373 К	Driver Length		60 "
Primary Driver Gas	He + Ar	Insert Length		50"
Primary Driven Gas	Ar + TFE	Driver Diameter		1"

Shock No.	Date	File name	Reaction Time - 80% [s]	P5 - Max [psi]	P5-80% [psi]	P5 - Max [atm]	Tailoring Gas -Ar [psi]	Driver pressure - P4 [psi]	Driven Pressure - P1 [psi]	Velocity [ms-1]	Ideal Temperature - T5 [K]
4	14-Dec-17	12142017_TFE_01	0.002940	412.7	308.32	28.1	120	590	27.3	709.19	1245.79
7		12142017_TFE_04	0.003095	308.1	228.80	21.0	120	465	22.1	691.83	1192.18
10	15-Dec-17	12152017_TFE_02	0.003403	287.2	216.56	19.5	120	440	16.5	709.95	1248.18
11		12152017_TFE_03	0.003234	336.7	255.68	22.9	125	500	17.1	728.08	1305.54
13		12152017_TFE_05	0.003174	348.4	259.36	23.7	125	555	24.2	715.18	1264.60
14		12152017_TFE_06	0.003296	291.0	221.44	19.8	120	465	14.2	749.36	1374.60
15	18-Dec-17	12182017_TFE_01	0.003260	304.0	227.60	20.7	125	480	19.5	698.55	1212.80
16		12182017_TFE_02	0.003302	326.4	248.40	22.2	125	480	15.9	740.01	1344.02
18		12182017_TFE_04	0.003094	334.2	255.68	22.7	125	525	14.6	764.44	1424.63
20		12182017_TFE_06	0.003429	279.2	212.88	19.0	120	440	13.1	747.69	1369.11
21	19-Dec-17	12192017_TFE_01	0.002965	334.0	255.68	22.7	125	515	14.4	763.27	1420.71
24		12192017_TFE_04	0.003183	358.0	272.88	24.4	130	555	16.9	747.53	1368.57
28	20-Dec-17	12202017_TFE_02	0.003741	289.2	215.36	19.7	140	470	20.0	682.69	1164.39
29		12202017_TFE_03	0.003510	286.7	215.36	19.5	130	475	17.5	717.66	1272.41
31		12202017_TFE_05	0.003387	351.4	267.92	23.9	140	550	16.5	741.00	1347.23
32	18-Jan-18	01182018_TFE_01	0.003092	375.9	286.32	25.6	130	545	18.0	737.79	1336.81

Mixture Details

	Pvac	0.0374	Torr			Concentration		207.75 ppm		ppm			
+	Pfuel	5.28	Torr	4	ŀ	PNe	0	Torr		+	PAr	35.21	atm
=	Ptotal	33.44	atm	[Next Day]									

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VITA

Name	Jai M. Mehta
Education	Diploma in Mechanical Engineering, Shri Bhagubhai Mafatlal Polytechnic, Mumbai-India ,2013
	Bachelor of Engineering (B.E.), Mechanical Engineering, University of Mumbai, Mumbai-India, 2016
	Master of Science (M.S.) , Mechanical Engineering , University of Illinois at Chicago , Chicago-Illinois , 2018
Work Experience	Graduate Research Assistant, UIC – High Pressure Shock Tube Laboratory, University of Illinois at Chicago, Chicago - Illinois, 2017-2018
	Engineering Intern – Transportation Engineering, Brihanmumbai Electric Supply & Transport Undertaking, Mumbai-India, 2012-2013
	Intern – Engine Overhauling Division, <i>Air India Ltd</i> , Mumbai-India, 2011
Membership	Society of Automotive Engineers (SAE), Formula SAE team member (2014-2016)
	The American Society of Heating, Refrigeration and Air Conditioning (ASHRAE)