Driver-gas Tailoring For Test-time Extension Using Unconventional Driver Mixtures

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DRIVER-GAS TAILORING FOR TEST-TIME EXTENSION USING UNCONVENTIONAL DRIVER MIXTURES

by

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B.S. University of Florida, 2004

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in the Department of Mechanical, Materials and Aerospace Engineering in the College of Engineering and Computer Science at the University of Central Florida Orlando, Florida

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ABSTRACT

To study combustion chemistry at low temperatures in a shock tube, it is of great importance to increase experimental test times, and this can be done by tailoring the interface between the driver and driven gases. Using unconventional driver-gas tailoring with the assistance of tailoring curves, shock-tube test times were increased from 1 to 15 ms for reflected-shock temperatures below 1000 K. Provided in this thesis is the introduction of tailoring curves, produced from a 1-D perfect gas model for a wide range of driver gases and the production and demonstration of successful driver mixtures containing helium combined with either propane or carbon dioxide. The He/CO₂ and He/C₃H₈ driver mixtures provide a unique way to produce a tailored interface and, hence, longer test times, when facility modification is not an option. The tailoring curves can be used to guide future applications of this technique to other configurations. Nonreacting validation experiments using driver mixtures identified from the tailoring curves were performed over a range of reflected-shock temperatures from approximately 800 to 1400 K, and some examples of ignition-time experiments that could not have otherwise been performed are presented.
Dedicated to my Wife, my Family, and Dearest Friends and Professors
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LIST OF ABBREVIATIONS

\[ a: \] Sound velocity, \( m/s \)

\[ A: \] Surface area, \( m^2 \)

\[ c_p: \] Constant pressure specific heat, \( J/kg-K \)

\[ c_v: \] Constant volume specific heat, \( J/kg-K \)

\[ CS: \] Contact Surface

\[ C+: \] Right-running characteristic line

\[ C-: \] Left-running characteristic line

\[ D_{23}: \] Binary diffusion coefficient across the contact surface, \( m^2/s \)

\[ e: \] Specific internal energy, \( J/kg \)

\[ h: \] Specific enthalpy, \( J/kg \)

\[ HE: \] Head expansion wave

\[ i: \] \( i^{th} \) component

\[ IS: \] Incident shock wave

\[ k: \] Thermal conductivity, \( W/m-K \)

\[ L: \] Length, \( m \)

\[ MW: \] Molecular weight, \( g/mol \)

\[ p: \] Pressure, \( atm \)

\[ R: \] Gas constant, \( J/kg-K \)

\[ R_U: \] Universal gas constant, \( J/kmol-K \)

\[ RS: \] Reflected shock wave

\[ t: \] Time, \( ms \)
$T$: Temperature, $K$

$TE$: Tail expansion wave

$u$: Absolute gas velocity, $m/s$

$V$: Relative gas velocity, $m/s$

$v$: Volume, $m^3$

$W$: Shock wave velocity, $m/s$

$X$: Mole fraction

$γ$: Specific heat ratio

$δ$: Hydrodynamic boundary layer growth, $cm$

$δ_{cs}$: Contact surface growth, $cm$

$δ_{r}$: Thermal penetration depth, $cm$

1: Initial state of driven gas

2: Post incident shock state of driven gas

3: Post incident expansion state of driver gas

4: Initial state of driver gas

5: Post reflected shock state of driven gas or test state

6: Post reflected expansion state of driver gas

7: Under-tailored or over-tailored state of driven gas

8: Post reflected shock state of driver gas
CHAPTER ONE: INTRODUCTION

A shock tube is a long tube having a high-pressure driver section and a low-pressure driven section, separated by a diaphragm, see Fig. 1. When the pressure difference across the diaphragm is large enough to cause it to rupture, the high-pressure driver gases will push through the low-pressure driven gases like a piston which will then generate a shock wave almost instantly. This incident shock wave propagates to the end of the driven section while heating and compressing the driven gases. After reaching the endwall, the reflected shock causes additional heating and compression of the driven gases while leaving it stagnant. It is this high pressure, high temperature, stagnant region that is the region of observation, or test region.

![Diagram of shock tube](image)

Figure 1: The shock tube for generating shock waves
Figure 2: The generated shock wave is used to compress and heat the test gas. (a) The incident shock wave travels to the endwall. (b) The reflected shock wave travels away from the endwall leaving the test gas stagnant and at high temperature and pressure.

Through thermodynamic and gas dynamic relationships, the generated shock wave can be manipulated to reproduce any temperature and pressure in the test region. For this reason, shock tubes are commonly employed to study chemical kinetics and other combustion phenomena, and they can model almost any combustion system: automotive
engines, diesel engines, rockets, and gas turbines (see Fig. 3) are a few examples. Experimental test times in chemical kinetics shock tubes are often on the order of 1 ms. At low and intermediate temperatures, between 800 K and 1400 K, reactions are slow and auto-ignition times can be several milliseconds. In particular, auto-ignition in gas turbine premixers is of great concern since the addition of synthetic fuel blends accelerates the very slow ignition delay time of methane from 20+ ms to less than 10 ms resulting in reactions in the premixed circuit before the main combustor, see Fig. 4.

Figure 3: Gas turbine engine for power generation
Conventional shock tubes have driven-to-driver lengths of about 3 or greater, and helium is typically used as the driver gas. Helium is very efficient for producing strong shocks because it has a very low molecular weight\(^1\). However, large sound speeds lead to fast-propagating expansion waves that ultimately reduce test times. One way to decrease the sound speed is to tailor the driver gas by mixing He with heavier gases. Tailoring with He/N\(_2\) or He/Ar mixtures in the driver may not work for the conventional shock tube if the driver is too short, see Fig. 5, unless the driver length is increased or the driven length is reduced. If facility modification is not an option, then for true tailoring to occur, one must tailor with heavier gases having smaller specific heat ratios.
Figure 5: Shock Tube Configurations (a) Conventional: driver-to driven length = 3+ (b) Traditional Tailoring: ideal driver-to driven length = 1 (c) Unconventional Tailoring: conventional geometry using never before seen driver-gas combinations (i.e., exotic gases)
The shock tube used herein\(^2\) has a fixed geometry wherein the driver length (3.5 m) is relatively short compared to the driven length (10.7 m), and it is the reflected head expansion wave that reaches the contact surface before the reflected shock wave. If the driver is too short, such that tailored compositions of He/N\(_2\) or He/Ar in the driver will not expose the contact surface to the reflected shock, then true tailoring cannot be achieved. Since expansion waves travel at the local speed of sound of the gas they occupy, their speeds can be reduced significantly in the driver by mixing helium with heavier gases that have smaller specific heat ratios. With this in mind, and from 1-D perfect gas assumptions, tailoring curves were developed as a guide for a better physical understanding of the physics of a tailored condition in a shock tube. Tailoring curves are unique in that for each test temperature and test gas, there is only one tailoring curve. Yet, tailoring curves show that there are infinite driver-gas combinations that can give a tailored condition in a shock tube. With the assistance of the tailoring curves, unconventional driver-gas tailoring was developed and demonstrated.

Provided in this thesis is a review of the appropriate gas dynamics that limit the test time and allow for tailoring, followed by a description of the 1-D model utilized for the selection of candidate driver-gas mixtures. The results of experiments demonstrating longer test times in driven mixtures without reacting species are presented, followed by some typical ignition experiments with longer ignition delay times.
CHAPTER TWO: LITERATURE REVIEW AND BACKGROUND

For many years, shock-tube flows have been of great interest in the fields of engineering, physics, and chemistry. There have been considerable studies dealing with the non-ideal fluid flow in shock tubes such as shock attenuation, contact surface phenomena, and boundary layer effects. Driver-gas tailoring in shock tubes has also been studied for quite some time. Tailoring is used in many applications of research. For example, tailoring is used for increasing experimental test times to study ignition times related to gas turbine and diesel combustion using both gas mixture and spray injection configurations. For hypersonic aerodynamics studies, drivers use tailoring for better performance and longer test times. Details on driver-gas tailoring can be found in many references, for example Gaydon and Hurle, Glass and Sislian, and Nishida. However, most papers did not use gases other than N₂ or Ar for a driver mixture, particularly for combustion chemistry applications. As mentioned above, N₂ and Ar mixed with helium may not produce acceptable sound speeds for certain driver and driven hardware that are fixed in size. In cases where one can design or change the driver and driven-section lengths, tailoring with gases other than He/N₂ or He/Ar can lead to even longer test times behind the reflected shock wave. Further details are provided below.
2.1 Shock Tubes for Combustion Experiments

For shock-tube combustion experiments behind reflected shock waves, the shock-tube test time, $t_{AB}$, is defined as the time between when the reflected shock wave leaves the endwall (A) to the time when the next wave, a compression or expansion wave, reaches the end wall (B), such that the test pressure and temperature both increase or decrease, respectively. In practice, strong incident shock waves are desired for high test temperatures ($T_5$). For this reason, many shock tubes use helium as a driver gas. Figure 6 is a wave (or x-t) diagram showing the thermodynamic regions for a tailored condition in an ideal shock tube. The assumptions for an ideal shock tube will be defined in the next section. In the usual fashion, "tailored" herein means that there is no pressure discontinuity at point "P" where the reflected shock collides with the contact surface, i.e., $p_8 = p_5$. As a result, the contact surface is stationary, and there is no net flow to accompany the formation of new waves to travel to the endwall.

![X-t diagram for a tailored condition in an ideal shock tube](image)

Figure 6: X-t diagram for a tailored condition in an ideal shock tube
When the diaphragm of a shock tube breaks, it delivers a series of compression waves (right running characteristic lines) traveling at the local sound speeds into the driven section. The local sound speed of a gas is defined as

\[ a = \sqrt{\frac{\gamma R_u}{MW}T} \]  

Since compression waves heats the gas it propagates in, the head compression wave is slower than the tail compression wave. When any one of the compression waves within the series reaches the next compression wave ahead, a shock wave is formed. After all compression waves have coalesced, the shock wave has achieved its full strength (maximum compression), see Fig. 7. The time required to generate a shock wave at maximum strength is much less than the time it takes for that same shock wave to reach the endwall. For practical shock tube applications, it is assumed that the full strength shock wave is formed instantaneously, and the expansion waves are centered at the origin.
Similarly, when the diaphragm breaks, it delivers a series of expansion waves (left running characteristic lines) traveling at the local sound speeds into the driver section. Since expansion waves cool the gas they propagate in, the head expansion wave is faster than the tail expansion wave, see Fig. 7.

At an initial temperature of 298 K and helium as a driver gas, the head of the incident head expansion wave travels at 1016 m/s. It then hits the driver endwall where it bounces back at a lower speed and accelerates to a velocity greater than its incident velocity (due to the addition of the bulk flow) after it passes through the expansion fan. Ideally, for test temperatures, $T_s$, between 700 K and 1400 K, the interface between the driver and driven gases, or contact surface, travels at speeds of about 240 - 470 m/s in argon, and about 400 - 760 m/s in air. It is the thermodynamics of the driver and driven gases that determines the wave speeds, and the geometry of the shock tube determines the test times. If the driver section length is too short, or if the driven length is too long, the
reflected expansion head will reach the contact surface before the reflected shock wave and will end the shock tube test time as in Fig. 8a. Traditional driver-gas tailoring using He/N$_2$ will not work if the driver is still too short for the lower test temperatures of interest.

Since expansion waves travel at the local speed of sound of the gas they occupy, their speeds can be reduced significantly in the driver by mixing with heavy gases, hence postponing expansion-wave arrival at the test-section endwall, as shown in Fig. 8b for the case with a mixture of propane and helium in the driver. As mentioned above, the authors' shock tube has a relatively short driver section, so the purpose of this study was to increase the short-driver shock-tube test time.
Figure 8: Comparison between He and a mixture of C\textsubscript{3}H\textsubscript{8}-He in the driver gas of a conventional shock tube. Bath gas: Ar; driver L/driven L = 3\textsuperscript{+}. (a) Main expansion wave arrives at endwall first. Driver mixture: He (b) Head expansion wave arrival is delayed. Shock wave arrives at endwall first. Driver mixture: C\textsubscript{3}H\textsubscript{8} mixed with He
3.1 Analytical Model of a Shock Tube

Before performing any experiments, a gas dynamics model of the shock tube was developed using the following assumptions, or ideal shock-tube assumptions:

- Perfect gas
- Nonreacting flow
- One-dimensional flow
- Adiabatic flow
- No mass diffusion across the contact surface
- Two-wave approximation of method of characteristics
- Conservation Equations: Mass, Momentum, and Energy

3.1.1 Perfect Gas

The perfect gas assumption combines the assumptions of the ideal gas behavior (thermally perfect)

\[ p = \rho \left( \frac{R}{MW} \right) T \]

and constant specific heats (calorically perfect)

\[ \Delta h = c_p \Delta T \]

\[ \Delta e = c_v \Delta T \]
\[ \gamma = \frac{c_p}{c_v} = \text{const} \]

Eqn. 2 assumes that atoms and molecules have zero volume and have negligible attraction and/or repulsion forces acting between other atoms and molecules. Eqn. 2 does not hold validity at extremely high pressures (intermolecular forces are not negligible) and at low temperatures approaching saturation conditions (condensation).

Eqns. 3-5 assumes that the vibrational energy modes of the molecules are negligible compared to the translational and rotational energy modes. Consequently, there is no dissociation or ionization of the gas molecules. Unlike Eqn. 2, Eqns. 3-5 cannot hold validity at very high temperatures due to the molecular vibrations causing bonds to break apart.

3.1.2 Nonreacting

The assumption of nonreacting flow means that the chemical composition of the driver and driven gases are not changing. Gas dynamically speaking, nonreacting flow means the molecular weight of gases remain constant. This assumption holds valid for the expanded (cooled) driver gas and for the driven gas at the contact surface just after the passing of the reflected shock wave where the tailoring criteria is of concern.

3.1.3 One-Dimensional Flow

One-dimensional flow assumes that the thermodynamic properties of the driver and driven gases are a function of only the axial direction, \( x \), of the shock tube. In other words, there are no hydrodynamic boundary layers (inviscid) and no thermal boundary layers (adiabatic). Figure 9 shows the comparison between a one-dimensional
idealization of a shock tube versus a real, two-dimensional shock tube (by symmetry). Because a fluid adheres to solid surfaces (no slip), a hydrodynamic boundary layer begins in the driver between the head of the expansion wave and the incident shock wave. As a result of the no slip condition and by the law of mass conservation, shown in Fig. 9b, the fluid traveling in the direction from the driver to the driven is being squeezed and accelerated in the shock tube by the growing boundary layer. Also, shown in Fig. 9b, from the no slip condition and from the law of energy conservation, the shock wave attenuates as it is propagating.

For the test conditions of interest, 800-1400 K and 1-20 atm, shock tube boundary layer growth can be as large as about 2 cm\(^{10}\), as compared to the 16.2-cm inner diameter of the shock tube in this study. This can result in a significantly faster contact surface velocity than that predicted by 1-D assumption.
Figure 9: Comparison between a 1-D shock tube and a 2-D shock tube (a) 1-D: Properties are a function of $x$ and $t$ only (b) 2-D: Properties are a function of $x$, $r$ and $t$

3.1.4 Adiabatic Flow

Although the assumption of 1-D flow implies no radial heat exchange between the system (gases) and the surroundings (stainless steel shock tube), the addition of adiabatic flow assumes that there is no heat exchange between the shock-tube walls and the gases and there is no heat exchange across the thermodynamic regions.

Heat exchange does take place in a real shock tube, however, a significant amount of heat exchange takes a significant amount of time. Eqn. 6 defines the ratio of the fluid time scale to the heat transfer time scale.
For any real problem, there is no heat transfer across a planar shock wave. A shock wave is a few mean free paths thick allowing no side surface area for heat exchange, and there are no temperature gradients just ahead and behind the normal shock wave.

3.1.5 No Mass Diffusion across the Contact Surface

If there is no mass diffusion between the driver and driven gases (states 2 and 3), then there are no concentration gradients; i.e., the contact surface has zero thickness. In a real shock tube, there is turbulent mass diffusion with contributions being made in part by viscous effects and heat transfer from the hot driven gases to the driver gases. For a planar contact surface traveling for about 20 ms just before colliding with the reflected shock wave, the contact surface thickness is on the order of magnitude of about 10 cm, estimated from Eqn. 7 where the binary diffusion coefficient is calculated from kinetic theory\textsuperscript{20,21}.

$$\delta_{CS} \sim \sqrt{D_{23} t}$$

3.1.6 Two-Wave Approximation of Method of Characteristics

When the diaphragm of the shock tube breaks, the expansion waves are generated and travel to the driver endwall. When the head expansion wave reaches the driver endwall, it reflects back at a lower speed (cooler gas) and accelerates to a velocity greater
than its initial velocity after it passes through the expansion fan due to the addition of the bulk flow, see Fig. 10.

Figure 10: Centered expansion waves generated at the origin.

From the characteristic equations, the reflected head expansion wave is related to the contact surface speed and the initial sound speed in the driver from Eqn. 8

\[ a_3 = a_4 - \frac{(\gamma_4 - 1)}{2} u_3 \]  

Instead of considering the precise shape of every characteristic line (many waves must be assumed) in the expansion fan for a variety of experiments, the simplification of the method of characteristics neglects the acceleration (i.e., the shape) of the head and tail of the expansion waves as constant velocity (straight line), see Fig. 11. The two-wave
approximation of the method of characteristics considers only the head and tail of the incident expansion wave to determine the velocities of their reflected counterparts.

Figure 11: Two-wave approximation of the method of characteristics for the expansion wave.

3.1.7 Conservation Equations: Mass, Momentum, and Energy

In many high-speed flow applications, shock waves are the frame of reference and the analysis is a steady one. For observing chemical kinetics in a hot, stagnant gas behind the reflected shock wave, the tube is the frame of reference; the shock wave is moving, and the thermodynamic states are changing in space and time. For this reason, shock tube flows are unsteady. However, since the thermodynamic properties are independent of all reference frames, the relations between the fluid velocities relative to the planar shock still hold valid. Instead of having to consider unsteady terms in the conservation equations, simply substitute the difference between the absolute velocities in replace of
the relative velocities. The vector relation between the absolute and relative velocities across a normal shock wave is defined by

\[ \vec{V} = \vec{u} + \vec{W} \]

Figs. 12 and 13 demonstrate the substitution of Eqn. 8 into the normal shock relations, where the positive x-direction is to the right.

\[
\begin{align*}
\rho_1 V_1 &= \rho_2 V_2 \\
p_1 + \rho_1 V_1^2 &= p_2 + \rho_2 V_2^2 \\
h_1 + \frac{V_1^2}{2} &= h_2 + \frac{V_2^2}{2}
\end{align*}
\]

(a)
Mass: \[ \rho_1 W_s = \rho_2 (W_s - u_2) \]

Momentum: \[ p_1 + \rho_1 W_s^2 = p_2 + \rho_2 (W_s - u_2)^2 \]

Energy: \[ h_1 + \frac{W_s^2}{2} = h_2 + \frac{(W_s - u_2)^2}{2} \]

Figure 12: Normal incident shock wave equations (a) Steady reference frame: shock wave (b) Unsteady reference frame: shock tube

Mass: \[ \rho_2 V_2 = \rho_5 V_5 \]

Momentum: \[ p_2 + \rho_2 V_2^2 = p_5 + \rho_5 V_5^2 \]

Energy: \[ h_2 + \frac{V_2^2}{2} = h_5 + \frac{V_5^2}{2} \]
Rearranging the normal shock wave equations from Figs. 12 and 13 in terms of useful parameters for practical shock tube problems to get the following application equations

\[ M_S = \frac{W_S}{a_1} \]  

\[ u_2 = u_3 = \frac{2a_1}{\gamma_1 + 1} \left( M_S - \frac{1}{M_S} \right) \]  

\[ \frac{p_2}{p_1} = \frac{2\gamma_1 M_S^2 - (\gamma_1 - 1)}{\gamma_1 + 1} \]  

\[ \frac{T_2}{T_1} = \frac{\left( \gamma_1 M_S^2 - \frac{\gamma_1 - 1}{2} \left( \frac{\gamma_1 - 1}{2} M_S^2 + 1 \right) \right)}{\left( \frac{\gamma_1 + 1}{2} \right)^2 M_S^2} \]
From Eqn. 8 and noting the pressure and velocity at the interface are the same

\[ p_2 = p_3 \]

\[ u_2 = u_3 \]

The bridge between driver and driven gases take on the form

\[ \frac{p_4}{p_1} = \left[ 1 + \frac{2 \gamma_1}{\gamma_1 + 1} \left( M_S^2 - 1 \right) \right] \left[ 1 - \frac{\gamma_4 - 1}{\gamma_4 + 1} \left( a_S - \frac{1}{M_S} \right) \right]^{\frac{2 \gamma_4}{\gamma_4-1}} \]

After utilizing the ideal shock-tube assumptions, the difficulty of applying the continuity, momentum, and energy equations are significantly reduced. The application equations derived are all in terms of a measurable quantities: initial gas composition, initial temperature, initial pressure, and incident shock speed.

When analyzing the collision between the contact surface and the reflected shock wave, one must consider all three possible outcomes: under-tailored, over-tailored, and tailored condition, see Fig. 14. For the under-tailored interaction, Fig. 14a, the contact surface, similar to a piston, moves away from the endwall and expands the driven gas of state 5 via expansion waves. For the over-tailored interaction, Fig. 14b, the contact surface moves toward the endwall and compresses the driven gas via shock wave. The
tailored condition occurs when the contact surface comes to a complete stop after colliding with the reflected shock. Since the contact surface is no longer moving, it will cause no further compression or expansion, and no waves are generated to make known its presence.

**Under-Tailored:**

**Expansion Waves**

\[
\begin{align*}
\mathbf{u}_8 &= \mathbf{u}_7 < 0 \\
\mathbf{p}_8 &= \mathbf{p}_7 < \mathbf{p}_5
\end{align*}
\]

(a)

**Over-Tailoring:**

**Shock Wave**

\[
\begin{align*}
\mathbf{u}_8 &= \mathbf{u}_7 > 0 \\
\mathbf{p}_8 &= \mathbf{p}_7 > \mathbf{p}_5
\end{align*}
\]

(b)
Figure 14: Reflected shock wave – contact surface interaction (a) Under-tailored: expansion waves form (b) Over-tailored: shock wave forms (c) Tailored: No wave formation

From the time when the reflected shock wave reaches the contact surface and there onward, the wave interactions across 5, 7, and 8 are the same as the initial conditions when the diaphragm breaks. Following the same procedures from Figs. 12 and 13, applying the conservation equations, one can attack the tailoring condition from two sides; iterate the driver-gas composition starting with the over-tailored condition to achieve the tailored condition, or iterate the driver-gas composition starting with the under-tailored condition to achieve the tailored condition. The results will yield the perfect gas tailoring equation, as in Nishida

\[ \frac{\gamma_4 M W_3 T_3}{\gamma_1 M W_4 T_2} = \frac{1 + \frac{\gamma_4 + 1 p_5}{\gamma_4 - 1 p_2}}{1 + \frac{\gamma_1 + 1 p_5}{\gamma_1 - 1 p_2}} \left( \frac{2 \gamma_4}{\gamma_4 - 1} \right) \left( \frac{2}{\gamma_1 - 1} \right)^2 \]
For a specified bath-gas composition \((MW_1, \gamma_1)\), initial shock-tube temperatures, \(T_4\) and \(T_1\), and a test temperature of interest, \(T_5\) (varying \(W_s\) gives \(p_5/p_2\) which in turn gives \(T_5\)), then by iterating the driver-gas composition \((MW_4, \gamma_4)\) to obtain a tailoring condition.

### 3.2 Tailoring Curves

Recalling the definition of the sound speed of an ideal gas of a particular gas \(i\)

\[
a_i = \sqrt{\frac{\gamma_i R_T T}{MW_i}}
\]

The molecular weight and specific heat ratio of an ideal gas mixture can be determined using species mole fractions, \(X_i\), from

\[
MW_{Mix} = \sum_i X_i MW_i
\]

and

\[
\gamma = \frac{\left( \sum X_i \gamma_i \right)}{\left( \sum X_i \frac{\gamma_i}{\gamma_i - 1} \right)^{-1}}
\]

Table 1 list some common and unconventional driver gases and there sound speeds.
Using Eqns. 21 and 22, and properties from Table 1, gas mixture curves of He/Ar, He/N₂,
He/CO₂, He/R-116 (hexafluoroethane), and He/C₃H₈ are plotted in Fig. 15. All four
composition curves meet at helium, which is at $\gamma = 1.67$, $MW = 4$. 

<table>
<thead>
<tr>
<th></th>
<th>$\gamma$</th>
<th>MW</th>
<th>a(m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>He</td>
<td>1.67</td>
<td>4</td>
<td>1016</td>
</tr>
<tr>
<td>Ar</td>
<td>1.67</td>
<td>40</td>
<td>322</td>
</tr>
<tr>
<td>N₂</td>
<td>1.4</td>
<td>28</td>
<td>352</td>
</tr>
<tr>
<td>CO₂</td>
<td>1.29</td>
<td>44</td>
<td>269</td>
</tr>
<tr>
<td>R-116</td>
<td>1.08</td>
<td>138</td>
<td>139</td>
</tr>
<tr>
<td>C₃H₈</td>
<td>1.13</td>
<td>44</td>
<td>252</td>
</tr>
</tbody>
</table>

Table 1: Driver Gases and Sound Speeds at 298 K
Figure 15: Gas composition curves of He/Ar, He/N₂, He/CO₂, He/R-116, and He/C₃H₈.

For a specified bath gas \((MW_1, \gamma_1)\), initial shock-tube temperatures, \(T_4\) and \(T_1\), and a test temperature of interest, \(T_5\) (varying \(W_s\) gives \(p_5/p_2\) which in turn gives \(T_5\)), then by iterating the driver gas \((MW_4, \gamma_4)\) to satisfy the Eqn. 19, one can obtain a tailoring curve (shown as the solid lines in Fig. 16), where \(u_2 = u_3\) is the speed of the contact surface, and \(T_2\) and \(T_3\) are the temperatures of the gas in region 2 and 3, respectively. For a given set of conditions and a desired test temperature, there is a unique tailor curve that the driver gas must lie on to be tailored. Although unique, there are almost an infinite
number of possible driver gas mixtures that can satisfy a tailored condition, shown as the dashed lines on Fig. 16 for certain driver-gas mixtures composed of He and a heavier gas.

Figure 16: Gas composition curves (dashed) and tailoring curves (solid) for test temperatures \(T_3\) of 1400 K, 1200 K, 1000 K, and 800 K in Ar \((T_1 = T_4 = 298 \text{ K})\) under ideal shock-tube conditions.

In Fig. 16, the point of intersection of the tailor curves and the composition curves is the driver-gas composition that provides perfect gas tailoring for the corresponding test temperatures (i.e., incident-shock Mach number). The further down the driver gas is on
the tailor curve, the slower the local sound speeds. If the driver gas does not lie on the tailor curve, then there will be a pressure discontinuity at "P" (Fig. 6) where the reflected shock hits the contact surface. This discontinuity is immediately accounted for by the formation of an expansion wave (under-tailored; see Fig. 14a) or a shock wave (over-tailored; see Fig. 14b) at "P", depending on whether the pressure discontinuity is a sudden increase or decrease, respectively. If the driver gas is to the right of the tailor curve, a shock will form and travel to the test section. If the driver gas is to the left of the tailor curve, an expansion wave will form and travel to the test section.

Intuitively, one may figure that tailoring with a heavier gas will result in a slower expansion fan. However, this is not true when observing the location where the mixing curves intersect with the tailor curves, see Table 2. For example, although argon is heavier than nitrogen, to tailor at 1000 K in Ar requires about 23% Ar in He versus 45% N₂ in He. As a result, the sound speed of the driver is lower for the latter driver-gas mixture. This is also the case when comparing C₃H₈ with R-116. For a given driver-gas composition, too high of a test temperature (right side of tailor curve) will result in a shock wave formation, and too low of a test temperature (left side of tailor curve) will result in an expansion wave formation. Alternatively, for a desired test temperature, too much of the heavy gas will result in a shock formation at the contact surface, and too little of the heavy gas will result in an expansion wave formation. In Fig. 16, the left direction is the direction of increasing tailor test temperature.
Also, at lower test temperatures, the tailor curves are spaced further apart such that a small change in the driver-gas composition will result in a small change in the tailored test temperature. However, at higher test temperatures, the curves are closer together such that a small change in the driver-gas composition will result in a large change in the tailored test temperature. In other words, at low test temperatures, a driver-gas composition a little different from the tailored curve can lead to a slightly under-tailored or slightly over-tailored experiment (weak wave). At higher test temperatures, however, a driver-gas composition a little off from the tailored curve can lead to a highly under-tailored or highly over-tailored experiment (strong wave). Due to this fact, tailoring in practice is more difficult to achieve at higher test temperatures than at lower temperatures.

Preheating the driver gas (i.e., increasing $T_4$) will result in shifting the tailor curves to the right as shown in Fig. 17. This allows tailoring at much higher temperatures to be attainable. For example, 298 K helium in the driver gives a tailored condition for a

<table>
<thead>
<tr>
<th></th>
<th>$a$ (m/s)</th>
<th>Tailored $a_4$ (Driven: Ar)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ar</td>
<td>322</td>
<td>577 at 23% Ar + 77% He</td>
</tr>
<tr>
<td>$N_2$</td>
<td>352</td>
<td>516 at 42% $N_2$ + 58% He</td>
</tr>
<tr>
<td>CO$_2$</td>
<td>269</td>
<td>506 at 26% CO$_2$ + 74% He</td>
</tr>
<tr>
<td>R-116</td>
<td>139</td>
<td>467 at 9% R-116 + 91% He</td>
</tr>
<tr>
<td>C$_3$H$_8$</td>
<td>252</td>
<td>405 at 37% C$_3$H$_8$ + 63% He</td>
</tr>
</tbody>
</table>

Table 2: Driver Gases and Tailored Sound Speeds at 1000 K
test temperature of 3277 K (3.74 Mach number) in argon, ideally. Helium at 500 K gives a tailored condition for a test temperature of 5582 K (4.93 Mach number) in argon, ideally. For a given driven gas with initial temperature, shock-tube tailoring at the hottest temperatures is done by using heated hydrogen ($MW = 2, \gamma = 1.4$) as the driver gas since it is to the left of helium$^{8,14}$.

Figure 17: Tailoring curves for test temperatures ($T_3$) of 1400 K, 1200 K, 1000 K, and 800 K in Air (dotted), and Ar (solid: $T_1 = T_4 = 298$, dash dot dot: $T_1 = 298$ K, $T_4 = 500$ K) under ideal shock-tube conditions
If air (or N\textsubscript{2}) were used as the driven gas, it can be determined that the tailor curves in air are to the left of those for argon, see Fig. 17. As a result, there is much less of the heavy gas required to produce a tailored condition in air. For a 1000-K run in air, a tailored condition is 8% Ar in He, as compared to the same test temperature in argon having 23% Ar in He. Therefore, for a particular tailored test temperature, using argon instead of air for the driven gas will result in slower expansion waves in the driver gas.

Another way, and possibly a more convenient way, of looking at the tailoring curves is to look at a particular driver-gas combination as a function of the test temperature of interest. Figure 18 shows five gas-specific tailor curves: Ar, N\textsubscript{2}, CO\textsubscript{2}, R-116, and C\textsubscript{3}H\textsubscript{8} mixed in helium via molar percent as a function of the test temperature in Ar. Again, for a given driver-gas composition, too high of a test temperature (right side of tailor curve) will result in a shock wave formation, and too low of a test temperature (left side of tailor curve) will result in an expansion wave formation. Alternatively, for a desired test temperature, too much of the heavy gas (above the tailor curve) results in a shock formation at the contact surface, and too little of the heavy gas (below the tailor curve) will result in an expansion wave formation.

Similar to the results in Fig. 17, it can be shown that preheating the driver gas will shift the tailor curves in Fig. 18 up, and the tailor curves in air are below those of argon. Note that the slopes of the tailor curves in Fig. 18 decrease with higher test temperatures. This means, just like in Fig. 16, that at low test temperatures, a small change in the driver-gas composition will result in a small change in the tailored test temperature, and at high test temperatures, a small change in the driver-gas composition will result in a large change in the tailored test temperature. This again shows that tailoring is more sensitive at higher test temperatures.
Figure 18: Gas-specific tailoring curves for the driver-gas combinations of $N_2$, $C_3H_8$, $CO_2$, Ar, and R-116 mixed in helium (molar percent) as a function of the test temperature in Ar ($T_1 = T_4 = 298$ K) under ideal shock-tube conditions.

3.3 Experimental Facility

The current study utilized a stainless steel shock tube having a 3.5-m-long driver with a 7.62-cm inner diameter and a 10.7-m-long driven section with a 16.2-cm inner diameter$^2$, see Fig. 19. Sidewall pressures were measured with a Kistler 603B1 piezoelectric transducer, and endwall pressures were measured by a PCB 134A transducer. The incident shock speed was monitored with five PCB P113A pressure...
transducers and four Fluke model PM6666 time-interval counters. From those measurements, reflected-shock test properties were calculated using the standard 1-D shock-tube relations and the Sandia thermodynamic database\textsuperscript{22}. Further information on the facility, instrumentation, and procedure is provided in Petersen et al.\textsuperscript{2,23}

![Image of shock tube setup](image)

Figure 19: Gasdynamics and combustion experiments are performed in a shock tube

For the nonreacting experiments in this study, ultra high purity (UHP) argon was used as the sole test gas. Reacting mixtures using high-purity H\textsubscript{2} and UHP O\textsubscript{2} in stoichiometric proportion were diluted in 95% argon. Research-grade He, UHP CO\textsubscript{2}, and research-grade propane were used for the driver-gas mixtures, which were prepared either manometrically in a 0.0314-m\textsuperscript{3} tank or in the driver section itself, see Fig. 20. Dalton’s law states that

\[ P_{\text{Total}} = P_A + P_B + P_C + ... \]
Figure 20: The driver gas is prepared manometrically using Dalton’s law of partial pressures.
4.1 Nonreacting Model

Before performing any shock-tube experiments, the application equations derived from the ideal shock-tube model were used to develop wave diagrams in order to predict the wave interactions and the experimental test time. Table 3 lists tailored driver-gas compositions at 1000 K in Ar and there predicted test times.

<table>
<thead>
<tr>
<th>Gas</th>
<th>Tailored $a_4$ (Driven: Ar)</th>
<th>Model Test Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ar</td>
<td>577 at 23% Ar + 77% He</td>
<td>7 ms</td>
</tr>
<tr>
<td>N₂</td>
<td>516 at 42% N₂ + 58% He</td>
<td>9 ms</td>
</tr>
<tr>
<td>CO₂</td>
<td>506 at 26% CO₂ + 74% He</td>
<td>10 ms</td>
</tr>
<tr>
<td>R-116</td>
<td>467 at 9% R-116 + 91% He</td>
<td>12 ms</td>
</tr>
<tr>
<td>C₃H₈</td>
<td>405 at 37% C₃H₈ + 63% He</td>
<td>15 ms</td>
</tr>
</tbody>
</table>

Table 3: Tailored Driver-Gas Compositions and Predicted Test Times at 1000 K
\( T_5 = 1000 \text{ K} \)

**Driver:** He

**Driven:** Ar

---

\( T_5 = 1000 \text{ K} \)

**Driver:** 55\% He + 45\% \( \text{C}_3\text{H}_8 \)

**Driven:** Ar
$T_5 = 1300 \text{ K}$  \hspace{1cm} Driver: 80\% He + 20\% C_3H_8  \hspace{1cm} Driven: Ar

(c)

Figure 21: Comparison between He and a mixture of C_3H_8-He in an ideal shock tube. Bangladesh gas: Ar; driver L = 3.5 m, driven L = 10.7 m. (a) Main expansion wave arrives at endwall first. Driver mixture: He; $T_5 = 1000 \text{ K}$. (b) Weak shock wave arrives at endwall first. Driver mixture: 45\% C_3H_8 + 55\% He; $T_5 = 1000 \text{ K}$. (c) Expansion wave formed at the contact surface arrives at the endwall first. Driver mixture: 20\% C_3H_8 + 80\% He; $T_5 = 1300 \text{ K}$. 

4.2 Results – Nonreacting

Several experiments with He in the driver and Ar in the test section were performed to establish a baseline for untailored test times at lower temperatures. The pressure trace of a 932-K shock, displayed in Fig. 22a, gives a test time of approximately 1.0 millisecond. (Note that when higher test temperatures near 1400 - 2000 K are desired,
the test times are on the order of 2 to 3 ms.) When mixing the driver-gas helium with propane, the local sound speeds in regions 3 and 4 are reduced by more than half.

(a)
891 K, 0.87 atm
Driver: 45% C3H8 + 55% He
Driven: Ar

Compression Wave
Head Expansion Wave

8 ms
14.5 ms

(b)
Figure 22: Results from experiments; driver $L = 3.5$ m, driven $L = 10.7$ m. (a) Sidewall pressure trace with argon as the bath gas and helium as the driver gas. The test time is ended by the arrival of the main expansion wave as in Fig. 21a. (b) Endwall pressure trace with the addition of propane to helium driver gas at 891 K. The corresponding x-t diagram is provided in Fig. 21b. (c) Sidewall pressure trace with the addition of propane to helium driver gas at 1315 K. The corresponding x-t diagram is provided in Fig. 21c.
Figure 22b shows the delay of the reflected expansion head due to the addition of propane. By comparing Figs. 22a and 22b, the time difference in the expansion wave arrival at the endwall (or sidewall) test location is about 13.5 ms. Note that the practical test time in Fig. 22b is only about 8 ms due to the passing of the compression wave that was formed at the collision between the contact surface and the reflected shock wave. However, since the compression wave is rather weak, the pressure increase can be assumed negligible. If such a small change in pressure were important, suitable corrections to the test temperature can be made using an isentropic relation between $T_5$ and $p_5$, extending the test time until the arrival of the main expansion wave (14.5 ms).

It is important to note that a compression wave is observed in Fig. 22b, not a shock wave, since the pressure increases gradually. Under the assumptions of an ideal shock tube, the contact surface is a fine line. However, due to non-ideal effects, the contact surface has some thickness (concentration gradient). This means that that when the reflected shock crosses the contact surface, for the over-tailored condition, there will be a gradual increase in pressure, not a pressure discontinuity as predicted for the ideal case (see Fig. 21b), which will be corrected by a formation of compression waves traveling to the endwall. If the compression wave is strong (i.e., highly over-tailored), it can coalesce into a shock wave before approaching the endwall.

Figure 22c shows an expansion wave from the contact surface arriving at the endwall at about 5.5 ms, and the head expansion wave arriving at the endwall at about 8 ms. Since the test temperature in Fig. 22c, 1315 K, is hotter than the test temperature in Fig. 22b, 891 K, the gas dynamics are a little faster, hence the disturbances from the contact surface reaches the endwall quicker, 5.5 ms as compared to 8 ms, respectively.
The discontinuity in the slope of Fig. 22c reveals the arrival time of the head expansion wave.

In both Figs. 22b and 22c, the disturbances from the contact surface and the head expansion wave arrive at the endwall at an earlier time than that predicted under the assumptions of an ideal shock tube (see Fig. 21b and 21c, respectively). This is due to the non-ideal effects: the flow is accelerating behind the shock wave since it is being squeezed through the growing hydrodynamic boundary layer. Since the expansion or compression waves (formed at the contact surface-shock wave interaction) travel at the speed of sound into the stagnant test region, by comparing the arrival times between the model and the experiment, the real average contact surface speed can be determined and corrected for. For the shock tube used in this study, 1 atm experiments in Ar at 800 K to 1400 K has average contact surface speeds that are 40% to 25% faster, respectively, than those predicted by the 1-D model. Since the two-wave approximation of the method of characteristics neglects the curvature of the reflected head expansion wave, to accurately account for its arrival time requires a more detailed characteristics model (many waves) while using the corrected contact surface speed. Although real gas effects and viscous effects are present in the shock tube, the experimental tailored compositions are remarkably close to those predicted by the ideal shock-tube model.

Although heavy gases such as hydrocarbons and refrigerants have desirable thermodynamic properties for driver-gas tailoring, many have very low vapor pressures, which may limit the amount that can be used when high-pressure experiments are of interest. For high-pressure experiments, carbon dioxide may be a better alternative to propane. Or, one can have three (or more) gases in the driver such that driver-gas
composition is defined by the gas(es) with the lowest vapor pressure(s). Figure 23 shows a tailored condition at 792 K using 30% CO$_2$ in He as the driver gas.

Figure 23: A tailored endwall pressure trace with the addition of CO$_2$ to helium driver gas at 792 K and 0.865 atm. Test gas: 1% CH$_4$ + 1% C$_3$H$_8$ + 21% O$_2$ + 77% Ar (driver L = 3.5 m, driven L = 10.7 m)
4.3 Applications

Perfect gas tailoring curves were developed under the assumptions of a perfect gas and ideal conditions in a shock tube. Although real gases and other non-ideal effects are present in a shock tube, experimental tailored compositions are remarkably close to those predicted by the 1-D perfect gas model. Figure 24 shows the comparisons between the model and the experiments conducted in Figures 22b, 22c, and 23. The point of 45% C$_3$H$_8$ in He at 891K corresponds to the experiment from Figure 22b and it is just slightly above the C$_3$H$_8$ tailoring curve, which would result in a slightly over-tailored condition according to the model. This is in perfect agreement with the experiment from Figure 22b. The point of 20% C$_3$H$_8$ in He at 1315 K corresponds to the experiment from Figure 22c and it is slightly lower than the C$_3$H$_8$ tailoring curve, which would result in a under-tailored condition according to the model. This also is in perfect agreement with the experiment from Figure 22c. The point of 30% CO$_2$ in He at 792K corresponds to the experiment from Figure 23 and is just slightly below the CO$_2$ tailoring curve, which would result in an under-tailored condition according to the model. However, the experiment in Figure 23 is perfectly tailored. This is mainly due the deviation from constant specific heats in the ideal model and can simply be corrected by reducing the value of the specific heat ratio of the driven gas such that the tailored driver-gas composition of the model agrees with the experimental tailored driver-gas composition.
The procedure for developing perfect gas tailoring curves was outlined in Section 3. Tailoring curves bring about the physical understanding of driver-gas tailoring behind the mathematical iterations, hence reducing the amount of trial and error in experiments. All x-t diagrams with corresponding test times were developed using CAD software with a driver length of 3.5 m and a driven length of 10.7 m. To fully predict the
thermodynamics and gas dynamics in a particular shock tube, one must develop an x-t diagram using the continuity, momentum, and energy equations for one-dimensional shock waves. For the design of a new shock tube facility, given the restriction of size, one can choose the driver-to-driven ratio to obtain a maximum test time for a particular test temperature of interest. Again, for high-pressure experiments, carbon dioxide may be a better alternative to propane.

4.3 Results - Reacting

The driver-gas tailoring techniques outlined herein were used in recent chemical kinetics studies by the authors, and some examples are presented here for completeness – further details on the individual studies are presented in the cited works.

Figure 25 shows an endwall emission trace from a stoichiometric H\textsubscript{2}/O\textsubscript{2} mixture diluted in 95% argon at 885 K, utilizing a driver-gas composition of 35% CO\textsubscript{2} in He. Reaction progress was monitored by OH* chemiluminescence near 310 nm. Further details on the OH* measurements technique can be found in Petersen et al.\textsuperscript{23}. With an ignition time greater than 5 ms, this measurement could not have been obtained without mixing the driver with carbon dioxide. Figure 25 is shown here as an example of a chemistry experiment performed which the tailoring technique described herein. The complete study from with Fig. 25 was derived is presented in Hall and Petersen\textsuperscript{25}. 


Figure 25: Endwall pressure and emission traces at 885 K with 35% CO₂ + 65% He as the driver gas. Test gas: 3.4% H₂ + 1.7% O₂ + 94.9% Ar

Figure 26 shows a sidewall emission trace from a stoichiometric CH₄ + H₂/O₂ mixture diluted in 99% argon at 1334 K, utilizing an over-tailored driver-gas composition of 20% CO₂ in He as compared to an ideal tailored driver-gas composition of 16% CO₂ in helium. As a result of the extra addition of CO₂, Figure 17 shows a compression wave traveling to and from the endwall ending the 1.39 atm experiment at 4.5 ms. Reaction progress was monitored by CH⁺ chemiluminescence. With an ignition time greater than 2 ms, this measurement could not have been obtained without adding carbon dioxide to the driver. The complete study from with Fig. 26 was derived is presented in Hall^25.
Figure 26: Sidewall pressure and emission traces at 1334 K with 20% CO$_2$ + 80% He as the driver gas. Test gas: 0.2% CH$_4$ + 0.2% H$_2$ + 0.5% O$_2$ + 99.1% Ar

High-pressure, lower-temperature ignition experiments have also been performed as a result of the tailoring techniques herein. Figure 27 shows high-pressure endwall and CH$^*$ emission traces, at 803 K and 19.17 atm from a set of hydrocarbon/air ignition experiments$^{34}$. With a diaphragm breaking pressure ($P_4$) of 100 atm and the driver gas consisting of 34% CO$_2$ in He, the partial pressure of CO$_2$ is therefore 34 atm. Although 45% propane in the He driver would result in a tailored condition for the same test temperature and test gas, the partial pressure of propane in a 100-atm driver, which is about 45 atm, greatly exceeds its own vapor pressure, about 9 atm, so CO$_2$ was the better
gas to employ in these experiments. The ignition delay time for the lean methane-hydrocarbon-air ignition experiment shown in Fig. 27 is about 6 ms, which could not have been performed using pure helium as the driver gas. Further details on this special set of methane-hydrocarbon fuel blend experiments are presented elsewhere.  

![Graph](image)

Figure 27: Endwall pressure and emission traces for a high-pressure ignition experiment at 803 K and 19.2 atm with 34% CO\textsubscript{2} + 66% He as the driver gas. Test gas: 1% CH\textsubscript{4} + 1% C\textsubscript{5}H\textsubscript{12} + 21% O\textsubscript{2} + 77% Ar
CHAPTER FIVE: CONCLUSIONS AND RECOMMENDATIONS

To study combustion, it is of great importance to increase shock-tube test times. This increase can be done by tailoring the interface between the driver and driven gases. For drivers that are too short, a tailored mixture of He/Ar or He/N₂ will not slow down the expansion head enough to allow the reflected shock wave to reach the contact surface first. Instead of argon or nitrogen, heavier gases with smaller specific heat ratios, such as propane and carbon dioxide, were mixed in the driver in the present study. Using ideal gasdynamic assumptions for shock-tube flow, driver-gas tailoring curves were developed and plotted. Nonreacting shock-tube tests between 790 K and 1320 K in argon were shown. For the relatively short driver and using only helium, the test times were around 1 ms, as compared to having 45% propane or 30% CO₂ mixed with helium to give test times around 10 ms or greater. Also shown was a shock-tube ignition test of a stoichiometric H₂/O₂ reaction diluted in 95% argon and a high-pressure, fuel-lean CH₄/C₅H₁₂ mixture. With 34% CO₂ mixed in the driver, the observed ignition times for both experiments were greater than 5 ms, which could not have been obtained using helium in the driver alone. For very high pressures in the driver, carbon dioxide is a more suitable choice to propane due its higher vapor pressure.
LIST OF REFERENCES


