Effects of Helium and Carbon-Dioxide Dilutions on Hydrogen Jet Ignition in a Shock Tube

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1 Introduction

Research on hydrogen combustion is important for the mitigation of hydrogen accidental explosions [1]. Hydrogen is usually stored at high pressures and, in case there is an accidental leakage of a hydrogen jet from a high-pressure vessel into the atmosphere, there is formation of a shock wave and a contact surface [2]. The shock wave raises both pressure and temperature of the gas downstream of it. In addition, in the expansion process, the temperature of the hydrogen jet drops. Moreover, there is mixing between the hot air and the cold hydrogen at the contact surface, also referred to as diffusion layer [2,3]. Because hydrogen has a low Lewis number, i.e., high diffusion coefficient, it diffuses into the hot air region downstream of the shock wave [3]. Therefore, ignition should occur if the temperature rise caused by the chemical reactions is higher than the temperature drop caused by the jet expansion [2].

Hydrogen jet ignition is investigated experimentally in shock tubes [4]. A shock tube consists of a driver section, a driven section, and a diaphragm. The diaphragm can be a metal piece and it separates the driver and driven sections [5]. The driver section and driven section are also referred to as high-pressure chamber and low-pressure chamber, respectively. In a shock-tube experiment, as the driver section is filled with gas, the diaphragm bulges towards the driven section [6]. Eventually, the diaphragm ruptures and a jet propagates through the diaphragm opening into the driven section as the diaphragm tears and folds backwards [5]. In this process, compression waves form in the driven section, and eventually overtake each other and coalesce to form a shock front [5,6].

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The diaphragm rupture may also occur partially [7]. In these cases, the diameter of the diaphragm rupture, also referred to as diaphragm opening, is lower than the shock-tube diameter for a round cross-sectional area shock tube. Therefore, there is a diameter ratio between the diaphragm opening and the shock-tube cross section, \( d/D \), and an area ratio between the diaphragm opening and the shock-tube cross section, \( a/A \) [7].

A theoretical model was developed in [8] to calculate the gas properties throughout the shock tube in cases of a partially opened diaphragm. The model from [8] uses a discharge coefficient for flows past an orifice plate in order to account for stagnation pressure losses in the flow region near the diaphragm. Equations from the 1D simple shock-tube theory [9, 10] are also used in the model from [8]. Moreover, the model from [8] calculates the shock-wave Mach number at the distance of 3 \( D \) (three tube diameters) from the diaphragm and the gas properties downstream of the shock wave at this location. This location was chosen based on the fact that the shock wave becomes nearly planar at the distance of 3 \( D \) [7].

Initially, a discharge coefficient for incompressible flows past a concentric orifice plate with a vena contracta tap, \( C_{di} \), is calculated in the model from [8] in Equation 1 [11], where
\[
b = 0.00025 + 0.002325 (\sqrt{a/A} + 1.75 (a/A)^2 + 10 (a/A)^6 + 2 (D_H/a/A)^8);\]
\[
D_1 = (D_H/0.0254)^2 (a/A) + 0.01 (D_H/0.0254);\]
\[
\lambda = 1000 \sqrt{Re_H}.\]
In addition, \( D_H \) and \( Re_H \) are the hydraulic diameter of the driver section and the Reynolds number of the gas in the driver section, respectively. Equation 1 is applicable for
\[
D_H \geq 0.0429 \text{ m}, \quad Re_H > 10^4 \sqrt{a/A}, \quad \text{and} \quad 0.04 < a/A < 0.5625,\]
which imposes an applicability range in the model from [8].

\[
C_{di} = \left[ b \lambda + 0.5922 + 0.4252 \left( \frac{0.0006}{D_1} + \left( \frac{a}{A} \right)^2 + 1.25 \left( \frac{a}{A} \right)^8 \right) \right] \sqrt{1 - \left( \frac{a}{A} \right)^2} \quad (1)
\]

Moreover, the discharge coefficient for incompressible flows, calculated in Equation 1, is converted into a discharge coefficient for compressible flows in the model from [8] by using Equation 2 [12, 13], where
\[
f = 1/C_{di} - 1/(2C_{di}^2);\]
\[
r = P_b/P_0 = P_1/P_4;\]
\[
r_c = (2/(\gamma_4 + 1))^{\gamma_4/(\gamma_4 - 1)};\]
\[
r_1 = (r_c - r)/(r_c)^{1/\gamma_4};\]
\[
K_N = \gamma_4 (2/(\gamma_4 + 1))^{(\gamma_4 + 1)/(\gamma_4 - 1)};\]
\[
P_1 \text{ is the initial pressure of the driven gas; } P_4 \text{ is the initial pressure of the driver gas; and } \gamma_4 \text{ is the ratio of specific heats of the driver gas.}
\]

\[
C_{di} = \frac{1}{2f(r_c)^{1/\gamma_4}} \left[ 1 + \frac{r_1}{K_N^2} \right] - \sqrt{\left[ 1 + \frac{r_1}{K_N^2} \right]^2 - \left[ \frac{4(r_c)^2/\gamma_4(1-r)f}{K_N^2} \right]} \quad (2)
\]

The gas regions in the model from [8] are shown in Figure 1, where state 4 is the initial driver gas, state 3 is the expanded driver gas in the driver section, region 3a is the expanding driver gas in the driver section, \( j \) is the vena contracta region, region 2a is the expanding driver gas in the driven section, region 2b is the expanded driver gas in the driven section, state 2 is the gas downstream of the shock wave, and state 1 is the pre-shock gas. The model from [8] considers an isentropic expansion between state 3 and \( j \). Moreover, the model is only valid if the flow becomes sonic in \( j \); and the model assumes that the mass flow rate is constant between state 3, \( j \), and region 2b.

The model from [8] uses arbitrary values for \( a/A \); therefore, diaphragm physical properties are not accounted for in the calculation of \( a/A \) in [8]. The present work uses a new theoretical method to account for the effects of diaphragm properties on \( a/A \). Therefore, realistic values of \( a/A \) are calculated in the present work. Then, we investigate the effects of diaphragm thickness, driver-gas dilution, and driven-gas dilution on the gas region downstream of the shock wave, state 2. It is important to point out that chemical reactions, which may lead to ignition, occur in state 2 in shock-tube experiments. Therefore, it is important to investigate the gas properties in this region.
2 Methodology

A round cross-sectional-area shock tube with a diameter, \( D \), equal to 0.10 m is considered in the present work. The diaphragm material is nickel. The initial pressure of the driven gas (\( P_1 \)) is equal to 101325 Pa. The initial pressure ratio across the diaphragm (\( P_4/P_1 \)) is equal to 640. The initial temperature of both driver (\( T_4 \)) and driven (\( T_1 \)) gases is equal to 298 K. Moreover, the diaphragm material, \( P_1, P_4/P_1, T_4, \) and \( T_1 \) are the same in all cases investigated in the present work.

In order to investigate the effects of driver-gas dilution on the temperature in state 2 (\( T_2 \)), see Figure 1, different gas mixtures of hydrogen (\( H_2 \)), helium (\( He \)), and carbon dioxide (\( CO_2 \)) are considered as respective driver gases, as shown in Table 1, where \( X_{H_2}, X_{He}, \) and \( X_{CO_2} \) are the mole fractions of \( H_2, He, \) and \( CO_2, \) respectively, \( R_4 \) is the driver-gas constant in J/(kg·K), and \( c_4 \) is the speed of sound of the driver gas in m/s.

![Figure 1: Schematic of the model setup from [8].](image)

Table 1: Driver-gas properties, driven-gas properties, and 1D-theory solution.

<table>
<thead>
<tr>
<th>Driver gas</th>
<th>( X_{H_2} )</th>
<th>( X_{He} )</th>
<th>( X_{CO_2} )</th>
<th>( \gamma_1 )</th>
<th>( R_4 )</th>
<th>( c_4 )</th>
<th>Driven gas</th>
<th>( X_{Air} )</th>
<th>( X_{He} )</th>
<th>( X_{CO_2} )</th>
<th>( \gamma_1 )</th>
<th>( R_1 )</th>
<th>( c_1 )</th>
<th>( T_{2,1D} )</th>
<th>( M_{s,1D} )</th>
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<td>( H_2 )</td>
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<td>0.0</td>
<td>0.0</td>
<td>1.40</td>
<td>4124</td>
<td>1312</td>
<td>Air</td>
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<td>0.0</td>
<td>0.0</td>
<td>1.40</td>
<td>287</td>
<td>346</td>
<td>3018</td>
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<td>3930</td>
<td>1285</td>
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<td>0.0</td>
<td>1.42</td>
<td>3754</td>
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<td>1312</td>
<td>Air/He</td>
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<td>1312</td>
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<td>4124</td>
<td>1312</td>
<td>Air/CO_2</td>
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<td>341</td>
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<td>Air/CO_2</td>
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<td>4124</td>
<td>1312</td>
<td>Air/CO_2</td>
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<td>309</td>
<td>2974</td>
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</table>

The effects of driven-gas dilution on the temperature in state 2, see Figure 1, are investigated by considering different gas mixtures of air, He, and \( CO_2 \) as respective driven gases, as shown in Table 1, where \( X_{Air} \) is the mole fraction of air, \( \gamma_1 \) is the ratio of specific heats of the driven gas, \( R_1 \) is the driven-gas constant in J/(kg·K), and \( c_1 \) is the speed of sound of the driven gas in m/s. Moreover, the 1D-theory solution [10] for each case is shown in Table 1, where \( T_{2\,1D} \) is the gas temperature in state 2 and \( M_{s\,1D} \) is the shock-wave Mach number.

The extent of the diaphragm opening, i.e., the opening diameter (\( d \)), is calculated in Equation 3 [14],
where $t_d$ is the diaphragm thickness, $f_{ult}$ is the ultimate stress of the diaphragm material, and $\Delta P$ is the pressure difference between the driver gas and the driven gas that causes the diaphragm rupture, calculated as $\Delta P = P_4 - P_1$. The ultimate stress of nickel is 480 MPa [15].

\[
d = \frac{4t_df_{ult}}{\Delta P}
\]

Based on the values of $d$ calculated in Equation 3 and $D$; $a/A$ values are calculated as a function of $t_d$ and then implemented in the model from [8]. In shock-tube experiments, a rigid plate with an open area is placed on the diaphragm in order to control $a/A$ [7]. In this manner, the diaphragm opening area corresponds to the open area of the rigid plate; and there is a measurement of $P_4/P_1$ required to rupture the diaphragm [7].

3 Results

The results for $d/D$ for the driver gases and driven gases from Table 1 are shown in Figure 2. Because Equation 3 is not a function of the gas composition, the driver-gas and driven-gas dilutions do not affect the opening diameter, $d$. As a result, $d/D$ is the same at a specific $t_d$ for all cases from Table 1. Moreover, Figure 2 shows a linear increase in $d/D$ as $t_d$ increases, which is explained by the linear relationship between $t_d$ and $d$ in Equation 3.

Dilution of H$_2$ with He or CO$_2$ decreases the gas speed of sound when compared to pure H$_2$ (see Table 1). Therefore, respective driver-gas dilutions of H$_2$ with He and CO$_2$ produce weaker shocks than the case of pure H$_2$ as a driver gas, which is observed in $T_2|_{1D}$ and $M_s|_{1D}$ in Table 1 and in Figure 3 (Left) for He and Figure 3 (Right) for CO$_2$. For example, for $t_d = 2.5 \times 10^{-3}$ m, $T_2$ is decreased by 12% and 58% for $X_{He}=0.20$ and $X_{CO_2}=0.20$, respectively, when compared to the case of pure H$_2$ as a driver gas ($X_{He}=0.0$ and $X_{CO_2}=0.0$). However, the temperature drop caused by the driver-gas dilution gradually decreases with a reduction in $t_d$ (i.e., lower $a/A$ and therefore weaker shock). For example, for $t_d = 6.7 \times 10^{-4}$ m, $X_{He}=0.20$ and $X_{CO_2}=0.20$ lead to a temperature decrease by 5% and 37%, respectively, when compared to pure H$_2$ as a driver gas.

The respective driven-gas dilutions of air with He and CO$_2$ lead to changes in the speed of sound of the driven gas when compared to the case of pure air as a driven gas (see Table 1). For $X_{He}=0.40$, the speed of sound is higher than for the case of pure air as a driven gas by 27%. As a result, there is a temperature decrease by 7% at $t_d = 2.5 \times 10^{-3}$ m for $X_{He}=0.40$ when compared to the case of pure air ($X_{He}=0.0$).
as a driven gas, as shown in Figure 4 (Left). In regard to the driven-gas dilutions with CO₂, it is shown in Figure 4 (Right) that $T_2$ is reduced by up to 4% for $X_{CO_2}=0.40$ when compared to the case of pure air ($X_{CO_2}=0.0$) as a driven gas, which is explained by the fact that the speed of sound for this gas mixture is only lower than the speed of sound for pure air by 11%.

![Figure 3: Temperature profiles in state 2 as a function of $t_d$ for different driver gases. Left: H₂/He dilutions. Right: H₂/CO₂ dilutions.](image1)

![Figure 4: Temperature profiles in state 2 as a function of $t_d$ for different driven gases. Left: Air/He dilutions. Right: Air/CO₂ dilutions.](image2)

### 4 Conclusions

A new method was used in the present work in order to investigate theoretically the effects of the diaphragm properties, such as material and thickness, on the gas temperature in the region downstream of the shock wave ($T_2$) in a round cross-section shock tube with a diameter equal to 0.10 m and a partially opened nickel diaphragm at conditions of hydrogen jet ignition experiments (i.e., $P_4/P_1=640$). Furthermore, dilution effects of both driver gas and driven gas with He and CO₂ were investigated. It was found that a large dilution of air with He (i.e., $X_{He}=0.40$) as a driven gas can only reduce $T_2$ by 7% for a diaphragm with $t_d = 2.5 \times 10^{-3}$ m when compared to the case of pure air as a driven gas. On the other hand, driver-gas dilutions with He and CO₂ can lead to significant reductions in $T_2$ when compared to the case of pure H₂ as a driver gas. For example, for $t_d = 2.5 \times 10^{-3}$ m, $X_{He}=0.20$ and $X_{CO_2}=0.20$ lead to a reduction in $T_2$ by 12% and 58%, respectively, when compared to the case of pure
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H₂ as a driver gas. Future work will be carried out in order to compare the new method used in the present work with experimental results from the literature.

5 Acknowledgments

The authors would like to acknowledge the NRCN-CEA International Collaboration Research Fund and the Pazy Foundation for funding this research.

References


