Ignition Limits of Hydrogen-Diluted Jets in Shock Tubes with a Partially Opened Diaphragm

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1 Introduction

An accidental explosion may occur if there is an unintended release of a hydrogen jet from a high-pressure vessel into atmospheric air [1]. In the process of hydrogen release into atmospheric air, there is formation of a shock wave and a contact surface. The shock wave heats the downstream air and the contact surface is the location at which mixing between hot air and cold hydrogen occurs [2].

Hydrogen accidental explosions are investigated in shock tubes, which consist of a driver section, a driven section, and a diaphragm [1]. In a shock-tube experiment, the driver section is gradually filled with gas up to a pressure that leads to the diaphragm rupture. As the diaphragm ruptures, compression waves are formed in the driven section. The compression waves eventually overtake each other and coalesce in order to form a shock wave [3].

The diaphragm may be partially opened in a shock-tube experiment, which leads to a reduction in the resulting shock strength [4]. The shock strength (P_2/P_1) is the ratio of pressure downstream of the shock wave to pre-shock pressure. Shock strength is an important parameter because it is associated with the temperature in the gas region downstream of the shock wave (see state 2 in Fig. 1). Chemical reactions between hydrogen and air, which can lead to ignition, occur in the gas region downstream of the shock wave [2]. Note that high temperatures lead to high rates of chemical reactions, thereby increasing the probability of ignition [2].

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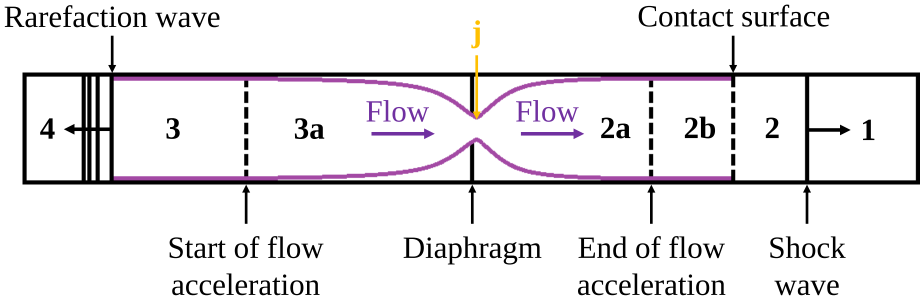

Figure 1: Schematic of the model from [5]. Adapted from [5].

Shock strength was investigated in a shock tube with a partially opened diaphragm in [4], where it was observed that the shock wave becomes nearly planar at the distance of $3D$ (i.e.; three tube diameters from the diaphragm). A theoretical model was developed in [5] to calculate the shock wave and gas properties in shock tubes with a partially opened diaphragm. A schematic of the gas states of the model from [5] is shown in Fig. 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, region j is the vena contracta, 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 region downstream of the shock wave, and state 1 is the pre-shock gas.

Although the model from [5] can calculate the gas properties in shock tubes with a partially opened diaphragm, it accounts for an instantaneous diaphragm opening, which occurs in shock tubes with a thin diaphragm. In hydrogen jet-ignition experiments in shock tubes, thicker diaphragms are required in order to deal with high pressures in the driver section. As a result, the gradual diaphragm rupture process needs to be accounted for and the ruptured diaphragm material can remain attached to the non-ruptured portion of the diaphragm, which imposes further stagnation pressure losses in the flow. Therefore, [6] developed another model, which calculates the losses due to the gradual diaphragm opening process in shock tubes with a partially opened diaphragm by presenting three different discharge coefficients as a function of a/A, which is the ratio of diaphragm opening area to driven-section cross-sectional area. Moreover, the model by [6] also predicts the absence or occurrence of hydrogen jet ignition in shock-tube experiments with a partially opened diaphragm by adapting an empirical correlation developed by [7], which was originally based on fully opened diaphragms, to the cases of partially opened diaphragms.

The model by [6] has been validated only against experimental results for pure H_2 as a driver gas. In other words, the model by [6] has never been applied to H_2 mixtures as driver gases. Therefore, in the present work, the model by [6] will be applied to different H_2 mixtures as driver gases and the effects of diluting H_2 with other gases will be shown and discussed.

2 Review of Model by [6]

In order to calculate the losses that occur during the gradual and partial diaphragm opening process in hydrogen jet-ignition shock-tube experiments, three discharge coefficient regimes are identified. The first regime occurs for $a/A \leq 0.125$, the second regime occurs for $0.125 < a/A < 0.25$, and the third regime occurs for $a/A \geq 0.25$. In the first regime, the ruptured portion of the diaphragm that remains attached to the orifice is negligible and therefore an abrupt flow expansion is considered between the opened diaphragm cross-sectional area and the driven-section cross-sectional area. In the third regime, the ruptured portion of the diaphragm material that remains attached to the orifice cannot be neglected as it imposes further restriction to flow propagation, which leads to the flow Mach number at the diaphragm cross-sectional area (M_d) being low and the jet becoming choked downstream (i.e.; $M_\mathrm{j} = 1.0$, see Fig. 2). In the second regime, there is a transition between the first and third regimes.

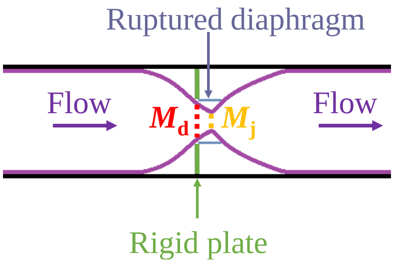

Figure 2: Schematic of the diaphragm rupture process in the model from [6]. Adapted from [6].

The discharge coefficient for incompressible flows (C_di) is calculated for the first, second, and third regimes in Eq. 1, Eq. 2, and Eq. 3, respectively, where γ_4 is the ratio of specific heats of the driver gas.

$$C_\mathrm{di} = \frac{a/A}{1-(a/A)} \tag{1}$$

$$C_\mathrm{di} = 0.3744\,(a/A) + 0.0961 \tag{2}$$

$$C_\mathrm{di} = M_\mathrm{d}\sqrt{\frac{2+\gamma_4}{2+\gamma_4 M_\mathrm{d}^2}} \tag{3}$$

Then, as shown in the model by [5], the discharge coefficient for incompressible flows (C_di) is converted into the discharge coefficient for compressible flows (C_d) in Eq. 4, where $f = 1/C_\mathrm{di} - 1/(2C_\mathrm{di}^2)$; $r = P_1/P_4$; $r_\mathrm{c} = (2/(\gamma_4+1))^{\gamma_4/(\gamma_4-1)}$; $r_1 = (r_\mathrm{c}-r)(r_\mathrm{c})^{1/\gamma_4}$; and $K_\mathrm{N}^2 = \gamma_4(2/(\gamma_4+1))^{(\gamma_4+1)/(\gamma_4-1)}$.

$$C_\mathrm{d} = \frac{1}{2f(r_\mathrm{c})^{1/\gamma_4}}\left\{\left[1+\frac{r_1}{K_\mathrm{N}^2}\right] - \sqrt{\left[1+\frac{r_1}{K_\mathrm{N}^2}\right]^2 - \left[\frac{4(r_\mathrm{c})^{2/\gamma_4}(1-r)f}{K_\mathrm{N}^2}\right]}\right\} \tag{4}$$

Shock strength is calculated in the model by [6] for each initial pressure ratio across the diaphragm (P_4/P_1) and area ratio (a/A). Then, absence or occurrence of ignition is calculated in a conservative manner in Eq. 5, where L is the driven-section tube length and D_eff is the driven-section effective diameter ($D_\mathrm{eff} = \sqrt{4A/\pi}$). Note that the model from [6] is applicable for any driven-section tube shape since D_eff is used in order to account for the tube cross-sectional area.

$$\left(\frac{A}{a}\right)^{0.25}\left(\frac{P_2/P_1 + 1.248}{4.550}\right) \geq 22.3\left(\frac{L}{D_\mathrm{eff}}\right)^{-0.58} \tag{5}$$

For shock tubes with a fully opened diaphragm, it was shown in [8] that ignition is likely to occur at the same shock strength (P_2/P_1) for different driver gas mixtures, such as pure H_2, $X_{H_2} = 0.975$ with $X_{N_2} = 0.025$, $X_{H_2} = 0.950$ with $X_{N_2} = 0.050$, and $X_{H_2} = 0.925$ with $X_{N_2} = 0.075$, where X_{H_2} and X_{N_2} are the mole fractions of H_2 and N_2, respectively. In addition, [9] showed that the same phenomenon occurs for experimental data from [10] for pure H_2, $X_{H_2} = 0.950$ with $X_{N_2} = 0.050$, and $X_{H_2} = 0.900$ with $X_{N_2} = 0.100$. Therefore, for $\gamma_4 \approx 1.40$, ignition is likely to occur at the same shock strength for different driver gas mixtures. Hence, Eq. 5 can be extended to hydrogen dilutions as respective driver gases provided that $\gamma_4 \approx 1.40$. In [9], it was shown that shock strength is the most important factor that affects ignition delay time. Therefore, a correlation that accounts for shock strength (i.e.; Eq. 5) to predict the occurrence or absence of ignition is used in the present work.

3 Gas Properties

In order to investigate effects of driver-gas dilution on the ignition limits (P_4/P_1), different gas mixtures of hydrogen (H_2), helium (He), nitrogen (N_2), and carbon dioxide (CO_2) are considered as respective driver gases, as shown in Table 1, where X_{He} and $X_{\mathrm{CO_2}}$ are the mole fractions of 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 for the initial driver-gas temperature (T_4) equal to 298 K.

Table 1: Driver-gas properties.

Driver gas	$X_{\mathrm{H_2}}$	X_{He}	$X_{\mathrm{N_2}}$	$X_{\mathrm{CO_2}}$	γ_4	R_4	c_4
H_2	1.00	0.00	0.00	0.00	1.40	4124	1312
H_2/He	0.95	0.05	0.00	0.00	1.41	3930	1285
H_2/N_2	0.95	0.00	0.05	0.00	1.40	2507	1023
H_2/CO_2	0.95	0.00	0.00	0.05	1.40	2020	918

In regards to the driven gas, air is considered as the driven gas in all the cases from the present work. The ratio of specific heats of the driven gas (γ_1) is equal to 1.40 and the gas constant of the driven gas (R_1) is equal to 287 J/(kg·K).

4 Results

Validation of the model by [6] was shown in the respective paper. Nevertheless, validation of the model by [6] against experimental results from [1] for $L/D_{\mathrm{eff}} = 13.29$ and the initial gas temperature ($T_1 = T_4$) equal to 300 K is shown again in Fig. 3 for the conservative ignition limits. In addition, the driver-gas dilution effects on the ignition limits are also shown in Fig. 3. Note that the model by [6] can predict the conservative ignition limit with a maximum relative error equal to 9% for $0.125 \leq a/A \leq 1.0$.

It is shown in Fig. 3 that a kink occurs at $a/A = 0.125$ and $a/A = 0.25$. These kinks occur because different discharge coefficient models (C_{di}) are used between $a/A < 0.125$ and $a/A > 0.125$, and between $a/A < 0.25$ and $a/A > 0.25$, respectively.

Moreover, the ignition limit decays rapidly for all driver-gas compositions and it eventually reaches a constant value at $a/A = 0.52$ for $X_{\mathrm{H_2}} = 1.00$ and $X_{\mathrm{He}} = 0.05$, $a/A = 0.46$ for $X_{\mathrm{N_2}} = 0.05$, and $a/A = 0.42$ for $X_{\mathrm{CO_2}} = 0.05$. Therefore, the ignition limit becomes independent of a/A at these conditions. It is also shown in Fig. 3 that the ignition limit increases as the speed of sound of the driver gas decreases. It is known that the shock strength of the produced shock wave decreases as the speed of sound of the driver gas decreases. Therefore, in order to achieve the required shock strength for ignition in Eq. 5, the initial pressure ratio across the diaphragm (P_4/P_1) increases [8, 10]. For a high value of P_4/P_1 to produce a weaker shock, a/A must decrease. Therefore, the value of a/A at which the ignition limit becomes constant (i.e.; reaches the same value as for $a/A = 1.0$) decreases as hydrogen is diluted as a driver gas (i.e.; the speed of sound decreases). The ignition limit increases by at least 3%, 36%, and 57% for $L/D_{\mathrm{eff}} = 13.29$ for $X_{\mathrm{He}} = 0.05$, $X_{\mathrm{N_2}} = 0.05$, and $X_{\mathrm{CO_2}} = 0.05$, respectively, when

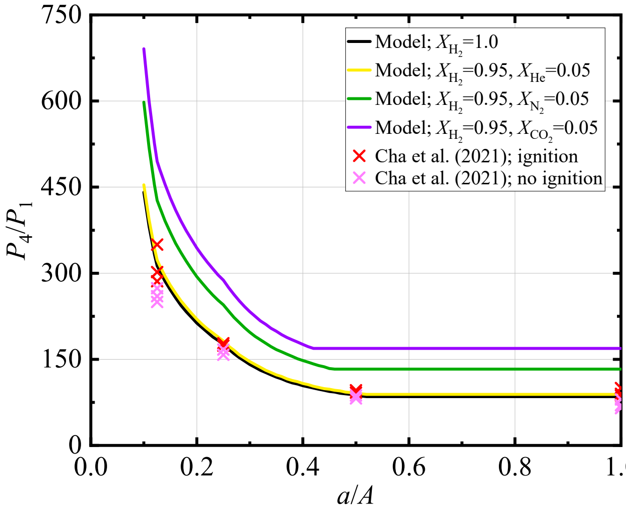

Figure 3: Ignition limits for $L/D_{\text{eff}} = 13.29$ for pure H_2 and H_2 dilutions as driver gases.

compared to $X_{H_2} = 1.00$. Note that the speed of sound for $X_{H_2} = 1.00$ and $X_{He} = 0.05$ are close to each other; therefore, the increase in ignition limit when diluting H_2 with 5% of He is negligible.

The cases for $L/D_{\text{eff}} = 5.0$ and $L/D_{\text{eff}} = 37.0$ for the initial gas temperature ($T_1 = T_4$) equal to 298 K are shown in Fig. 4 (Left) and Fig. 4 (Right), respectively. In regards to $L/D_{\text{eff}} = 5.0$, the ignition limit is increased by at least 4%, 46%, and 78% for $X_{He} = 0.05$, $X_{N_2} = 0.05$, and $X_{CO_2} = 0.05$, respectively, when compared to $X_{H_2} = 1.00$. In regards to $L/D_{\text{eff}} = 37.0$, the ignition limit is increased by at least 2%, 30%, and 47% for $X_{He} = 0.05$, $X_{N_2} = 0.05$, and $X_{CO_2} = 0.05$, respectively, when compared to $X_{H_2} = 1.00$.

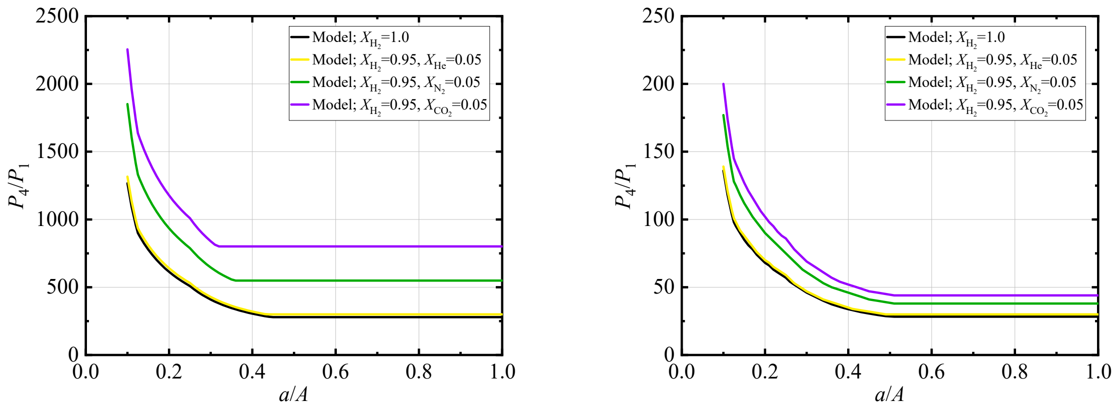

Figure 4: Ignition limits for pure H_2 and H_2 dilutions as driver gases. Left: $L/D_{\text{eff}} = 5.0$. Right: $L/D_{\text{eff}} = 37.0$.

5 Conclusions

The model by [6] for shock tubes with a partially opened diaphragm was used to quantify the ignition limits of hydrogen/inert-gas mixtures as driver gases for the first time based on the fact that the shock strength associated with ignition is the same for hydrogen/inert-gas mixtures, as previously shown in

[8], [9], and [10].

Moreover, the ignition limit eventually becomes independent of the area ratio (a/A) and the value of a/A at which the ignition limit becomes independent of a/A decreases as the speed of sound of the driver gas decreases for $L/D_{\text{eff}} = 5.0$ and $L/D_{\text{eff}} = 13.29$. On the other hand, the value of a/A at which the ignition limit becomes independent of a/A is nearly constant for $L/D_{\text{eff}} = 37.0$. The results shown in the present work can help with the design of shock-tube experiments for hydrogen jet ignition. Moreover, the results shown in the present work can help predict ignition in applications where there is release of pressurized hydrogen into tubing systems. In addition, the model shown in the present work can be applied to venting systems.

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