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Minimum diameters for CH₄/H₂-air mixtures: implications for natural gas cooktop burners

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Abstract

The minimum detonation diameter for methane (CH₄)/hydrogen (H₂)-air mixtures is numerically evaluated to assess detonation risks in cooktops designed to work with natural gas. A one-dimensional mathematical model that considers heat and friction losses for detonations propagating in pipes is used for that purpose. The initial conditions are selected to emulate the operation of a commercial cooktop working with different CH₄/H₂ blends. Results show that for H₂ content in the blend higher than 45 %, a conventional cooktop air-fuel mixer may pose a detonation hazard since the minimum detonation diameters predicted by the model are smaller than the diameter of the mixing tube (i.e., $d_{\min} < d_{\text{mixer}}$). Additionally, the individual effect of equivalence ratio, Φ , and hydrogen content, % H₂, in the fuel blend are evaluated separately. An increased risk of detonation is present for (i) CH₄/H₂-air mixtures with $\Phi \rightarrow 1$, and (ii) higher % H₂ content.

Keywords: CH₄/H₂ blend, minimum diameter, detonation, cooktop

1 Introduction

One of the strategies to reduce greenhouse gases emissions is the introduction of green hydrogen (H₂) into the world's energy matrix (Kong et al., 2021) but most current end-use equipment (e.g., industrial burners and residential/commercial heaters) is not designed to burn pure H₂. One of the interim strategies for a successful energy transition is to use natural gas (NG)/H₂ blends (Wojtowicz, 2019) on existing NG distribution networks. This provides the possibility of connecting H₂ producers with end-users in the short term and at a relatively low cost (Witkowski et al., 2018). The H₂ content (% H_{2,blend}) that could be safely added depends on the gas system of each country; Germany and The Netherlands have, to date, the highest authorized limits (% H_{2,blend} = 10 – 12) (Staffell et al., 2019).

The technology of cooktops designed to work with NG is quite simple (Figure 1). The fuel is injected from a small injector which increases the fuel discharge impulse, and in turn, draws air in from the surroundings resulting in a fuel-rich mixture. This mixture travels through the mixing tube to the combustion chamber, where ignition subsequently occurs and a partially premixed flame is generated. Cooktops are thus self-aspirating burners, similar to laboratory Bunsen burners. That is, part of the air (primary air) is mixed before combustion, and the rest (secondary air) is supplied by diffusion from the surroundings.

For safety reasons, the fuel concentration in the mixing tube must be higher than the upper flammability limit (UFL) in air to avoid accidental ignition and undesired flame propagation; the latter is known as flashback (Zhao et al., 2019a, Sayad et al., 2014). For this purpose, a primary air adjuster is used to control the amount of air that can be drawn in. The UFL of H₂ is higher (75 %vol) than that of CH₄ (15 %vol) which poses a safety hazard when increasing the content of H₂ in the fuel blend. If flashback occurs, the flame may potentially accelerate and transit to detonation, damaging the equipment and compromising the safety of end users.

Zhao et al. (2019b) studied the influence of H₂ addition to domestic natural gas burners, and evaluated the flashback limits for different CH₄/H₂ blends. The authors concluded that burners designed to burn NG are not suitable to work with % H_{2,blend} ≥ 20. Literature addressing detonation risks in CH₄/H₂ blends seems scarce. Faghih et al. (2016) numerically evaluated explosions characteristics of these

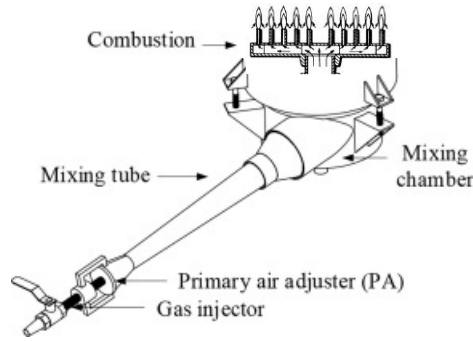


Fig. 1: Scheme of typical cooktop burner gas feed line including a gas injector, primary air adjuster, mixing tube/chamber and the combustion end. Adapted from (Chaelek et al., 2019).

blends based on the deflagration index and maximum pressure increase, which are important indicators to assess the potential damage resulting from accidental explosions. They concluded that for $\% \text{H}_{2,\text{blend}} > 70$, the deflagration index increases exponentially, and exhibits a strong/weak dependence on initial pressure/temperature. Pang and Gao (2015) evaluated the velocity deficit of $\text{CH}_4\text{-}2\text{H}_2\text{-}3\text{O}_2$, $\text{CH}_4\text{-H}_2\text{-}2.5\text{O}_2$, and $\text{CH}_4\text{-}4\text{H}_2\text{-}4\text{O}_2$ mixtures in a 36-mm inner diameter tube equipped with 2, 4, and 7.5-mm annular channels. A maximum velocity deficit of 7% from the ideal Chapman-Jouguet (CJ) velocity –mixture independent– was reported. Zhang et al. (2016) collected detonation cell size (λ) data for the same mixtures, concluding that detonation structure is irregular; a linear relationship between λ and the Zel’dovich-von Neumann-Döring (ZND) induction length, l_{ind} , was also reported.

A parameter of interest that could be applicable to NG burner design to avoid potential detonation hazard inside tubes is the minimum detonation diameter, d_{min} . It represents a limiting tube size below which detonation propagation is no longer possible. It is therefore good practice to have piping diameters that satisfy the later condition, i.e., $d < d_{\text{min}}$. Agafonov and Frolov (1994) performed a systematic study to derive a one-dimensional model capable of predicting d_{min} for pure and Ar/N_2 -diluted $\text{H}_2\text{-O}_2$ mixtures. Their results were found to be in agreement with available experimental data showing that an increasing $\% \text{H}_{2,\text{blend}}$ in the mixture results in a decrease in d_{min} . Gao et al. (2014) performed an experimental parametric study to determine d_{min} values for hydrocarbon-oxygen mixtures, i.e., acetylene (C_2H_2), propane (C_3H_8) and CH_4 , using polycarbonate tubes ($1.5 \text{ mm} < d < 50.8 \text{ mm}$). Their d_{min} results were shown to follow the $d_{\text{min}} = \lambda/3$ rule for the conditions evaluated. Surprisingly no study was found that reported d_{min} for CH_4/H_2 blends.

In the present work, the effect of the addition of H_2 to CH_4 on the minimum detonation diameter, d_{min} , is numerically evaluated. The paper is structured as follows. Section 2 introduces the physical model and the strategy followed to define the initial conditions for the simulations, which is based on the design and operating parameters of a commercial NG burner. Section 3 discusses the main results. Finally, section 4 presents the main conclusions applicable to the safe design of future cooktop burners working with CH_4/H_2 blends.

2 Methodology

2.1 Physical model

The flow is described by the compressible reactive Euler equations in a frame of reference attached to the shock. Here, the model presented in Veiga-López et al. (2022), which only included friction losses, is extended to account for heat losses. The system of equations thus reads:

$$\frac{d\rho}{dx} = -\frac{\rho}{w} \left[\frac{\dot{\sigma} + F_q - Q + (\eta - 1)F}{\eta} \right], \quad (1)$$

$$\frac{dw}{dx} = \left[\frac{\dot{\sigma} + F_q - Q + (\eta - 1)F}{\eta} \right], \quad (2)$$

$$\frac{dp}{dx} = -\rho w \left[\frac{\dot{\sigma} + F_q - Q - F}{\eta} \right], \quad (3)$$

$$\frac{dY_k}{dx} = \frac{1}{w} \frac{W_k \dot{\omega}_k}{\rho}, \quad k = 1, \dots, N. \quad (4)$$

ρ , w and $\dot{\sigma}$ sigma are the density, the axial velocity in the shock-attached frame and the thermicity. Y_k , W_k and $\dot{\omega}_k$ represent the mass fraction, molecular weight and net production/consumption rate of species k ; $\eta = 1 - M^2$ is the sonic parameter with $M = w/a_f$ the flow Mach number computed based on the frozen speed of sound, a_f . The functions F_q , F and Q are given by:

$$F_q = \frac{(\gamma - 1)}{a_f^2} c_f (D - w)^2 |D - w|; \quad F = c_f \left(\frac{D}{w} - 1 \right) |D - w|; \quad Q = \frac{(\gamma - 1)q}{a_f^2 \rho}, \quad (5)$$

with

$$q = \alpha c_p \rho |u| [c_p (T - T_w) + u^2/2]. \quad (6)$$

T , u , c_p and γ are the temperature, axial velocity in the laboratory frame, the specific heat at constant pressure of the gas and the ratio of specific heats; subscript w denotes conditions at the wall. In addition, the friction factor is defined as $c_f = P/(2A)\tilde{c}_f$, where P represents the perimeter of the tube, A its cross-sectional area, \tilde{c}_f denotes a dimensionless skin-friction coefficient of the rough walls of the tube. α is the momentum-heat loss similarity factor, $\alpha = 1$, reproduces the Reynolds analogy for heat and momentum losses which is characteristic of smooth tubes.

The friction factor and the actual tube diameters are related through the Blasius approximation for smooth tubes (Equation 7), which has been used successfully in previous works to analyze experimental trends (Kitano et al., 2009, Tsuboi et al., 2013). In Equation 7 μ_s and ρ_s are, respectively, the dynamic viscosity and density of the mixture at post-shock conditions in Pa-s and kg/m³, and u_s is the flow velocity measured relative to the shock wave, in m/s.

$$d = \left[\frac{0.6328}{c_f} \right]^{4/5} \left[\frac{\mu_s}{\rho_s u_s} \right]^{1/5} \quad (7)$$

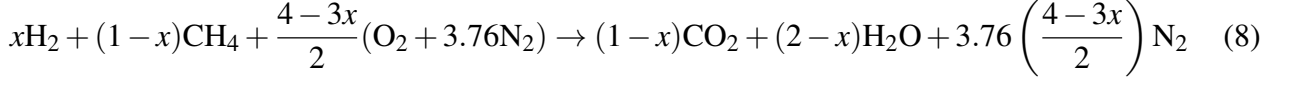
The output of system (1)-(7) are $D - d$ curves, that define the combination of detonation velocity (D) and tube diameter (d) that results in the steady propagation of a detonation wave. These curves exhibit a turning point, d_{\min} , that indicates the minimum tube diameter for which a steady solution exists for a given set of initial conditions; the d_{\min} value computed provides an estimate for detonation propagation limits. In Appendix A a comparison of the model's predictions with available experimental data for CH₄-O₂, H₂-O₂, and H₂-air mixtures is included.

2.2 Determination of initial conditions

2.2.1 Binary fuel mixture definition and upper flammability limit

The combustion reaction for a binary fuel mixture of CH₄/H₂ is shown in Equation 8. x denotes the mole fraction of H₂ in the blend ($x = n_{\text{H}_2}/n_{\text{blend}}$ where $n_{\text{blend}} = n_{\text{H}_2} + n_{\text{CH}_4}$); $x = 0$ is thus pure CH₄ and $x = 1$ pure H₂. Close inspection of Equation 8 reveals that as x increases, less air is required for

complete combustion of the mixture. Equation 9 expresses the equivalence ratio (Φ) of the mixture as a function of x and the mole fraction of fuel (X_{fuel}) and oxygen (X_{O_2}) in the reactive mixture.



$$\Phi = \frac{\left(\frac{n_{\text{fuel}}}{n_{\text{O}_2}}\right)_{\text{act}}}{\left(\frac{n_{\text{fuel}}}{n_{\text{O}_2}}\right)_{\text{stq}}} = \left(\frac{X_{\text{fuel}}}{X_{\text{O}_2}}\right) \left(\frac{4-3x}{2}\right) \quad (9)$$

Equation 10 shows the Le Chatelier's mixing rule (L'Chatelier, 1891, Mashuga and Crowl, 2004) used to calculate the upper flammability limit for fuel blends ($\text{UFL}_{\text{blend}}$) in air, where x_i and UFL_i are the mole fraction and upper flammability limit of each component in the blend ($i = \text{CH}_4$ and H_2), respectively. Figure 2 (a)-(b) show $\text{UFL}_{\text{blend}}$ and its corresponding equivalence ratio ($\Phi_{\text{UFL,blend}}$) as the content of H_2 in the mixture increases. Expectedly, the plots are bounded by $\text{UFL}_{\text{CH}_4} = 15\%$ ($\Phi_{\text{UFL,blend}} = 1.68$) for pure CH_4 and by $\text{UFL}_{\text{H}_2} = 75\%$ ($\Phi_{\text{UFL,blend}} = 7.12$) for pure H_2 .

$$\% \text{UFL}_{\text{blend}} = \frac{1}{\sum_{i=1}^k \frac{x_i}{\text{UFL}_i}} \times 100; \quad \sum_{i=1}^k \frac{x_i}{\text{UFL}_i} = \frac{x}{\text{UFL}_{\text{H}_2}} + \frac{1-x}{\text{UFL}_{\text{CH}_4}} \quad (10)$$

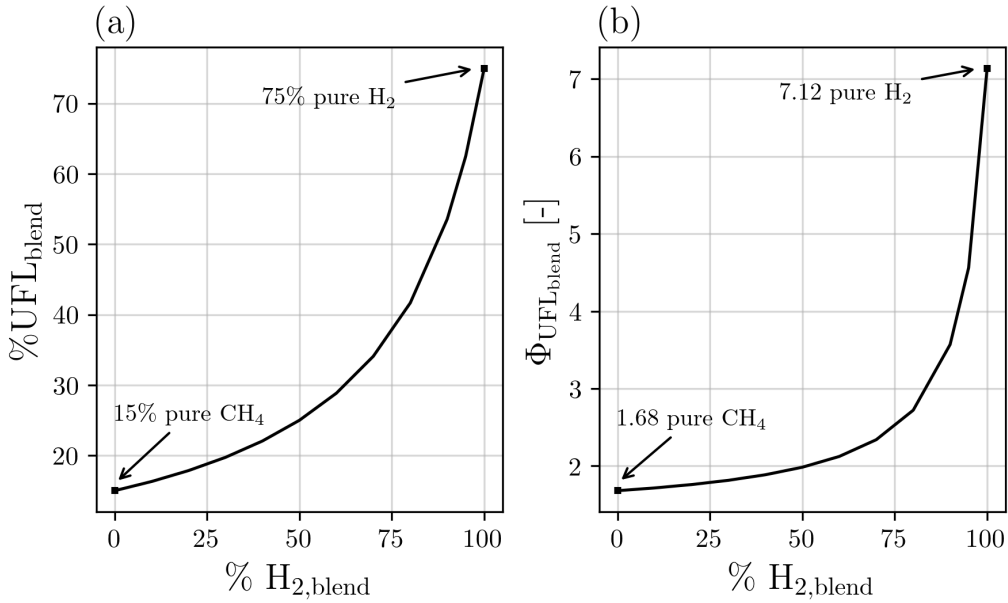


Fig. 2: (a) Upper flammability limit of the CH_4/H_2 blend in air and (b) equivalence ratio for the corresponding UFL of the blend, for different H_2 blend composition.

2.2.2 Commercial NG cooktop burner

The operating parameters of a commercial NG cooktop burner working at standard temperature and pressure (288 K and 101.325 kPa) are taken as the base case of our study. See Table 1.

In these burners, the fuel is injected through a nozzle whose diameter and supply pressure define the mass flow rate of fuel, \dot{m}_{fuel} . Equation 11 shows an expression derived using orifice discharge theory, where C is the injector discharge coefficient, A_{in} is the cross-sectional area of the injector, p_{in} is the gauge supply pressure and ρ_{fuel} is the fuel (CH_4/H_2) density. In the derivation of Equation 11, the

Table 1: Operational variables of a comercial NG cooktop

Parameter	Values	Units
Injector diameter (d_{in})	0.8	mm
Injection pressure (p_{in})	35	mbar-g
Discharge coefficient (C)	0.9	-
Mixer diameter (d_{mixer})	15.9	mm

flow is assumed to be adiabatic, incompressible, steady and subsonic; the latter assumption holds for injection pressures below 100 mbar-g (North American Manufacturing Company et al., 1997).

$$\dot{m}_{fuel} = CA_{in} \sqrt{2p_{in}\rho_{fuel}} \quad (11)$$

To avoid operational risks, such as accidental ignition and flame propagation before reaching the combustion chamber, it is common practice to ensure that the fuel-air mixture in the mixing tube (see Figure 1) is always above the upper flammability limit (UFL). To meet this condition, NG cooktop burners are equipped with a primary air adjuster as shown in Figure 1. The mass of air, \dot{m}_{air} , drawn in by the fuel jet (Equation 12) is computed using free jet theory; PA is the primary air adjuster opening, I is the fuel injection impulse, and ρ_{mix} is the density of the mixture which decreases considerably with increasing hydrogen content in the fuel blend $\%H_{2,blend}$. Equation 12 is derived via a momentum balance and assuming that: (i) the radial velocity and mass concentration profiles have the same shape at each axial section examined, and (ii) the jet forms an angle of $\sim 11^\circ$ with the horizontal in line with experimental observations (North American Manufacturing Company et al., 1997).

$$\dot{m}_{air} = 0.3 \cdot PA \sqrt{I\rho_{mix}} - \dot{m}_{fuel}; \quad I = \frac{\dot{m}_{fuel}^2}{\rho_{fuel}A_{in}} \quad (12)$$

PA is the burner parameter that needs being determined. To do so, the value $\Phi_{UFL,blend} = 1.68$, which corresponds to the design condition of a conventional NG burner is used. Figure 3 shows how the equivalence ratio of a pure CH_4 mixture (Φ_{mix,CH_4}) varies for different PA openings. As PA increases, more air is drawn into the mixing tube, which according to Equation 9 results in a decrease of Φ_{mix,CH_4} . For $\Phi_{mix,CH_4} = \Phi_{UFL,blend} = 1.68$, a $PA = 20$ mm is required; this value will be kept fixed for the remainder of the study.

2.2.3 Cases of practical interest

It is now possible to evaluate Φ_{mix} for different $\%H_{2,blend}$ and $PA = 20$ mm using the conditions listed in Table 1 (see Figure 4). Φ_{mix} decreases from 1.68 for $\%H_{2,blend} = 0$ to 1.27 for $\%H_{2,blend} = 88$. Further H_2 addition to 100% increases Φ_{mix} to 1.33. This behavior is due to the combined effect of increasing the fuel/air ratio and decreasing the air requirement for an increase of $\%H_{2,blend}$. Note that the values of Φ_{mix} obtained in Figure 4 are much lower than those shown in Figure 2 (b) for $\Phi_{UFL,blend}$, which represent unsafe operating conditions. To evaluate the burner performance under different $\% H_{2,blend}$, six cases are considered. These are indicated as circular markers in Figure 4, and are listed in Table 2 for clarity.

3 Results and discussion

The results presented in this section were obtained using GRI 3.0 (Smith et al., 1994) with thermodynamic data extended to cover the range of 300 K - 5000 K.

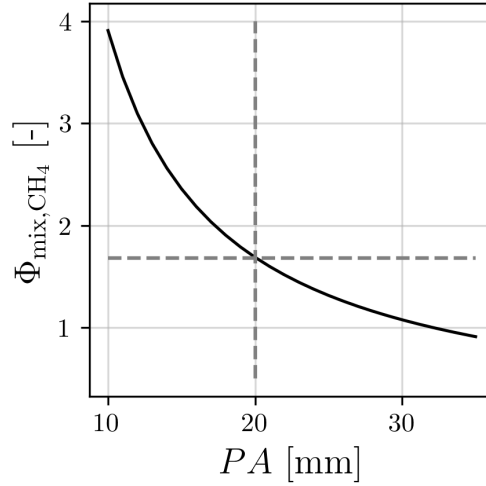


Fig. 3: Equivalence ratio for pure CH_4 in air as a function of the primary air opening using conditions of Table 1.

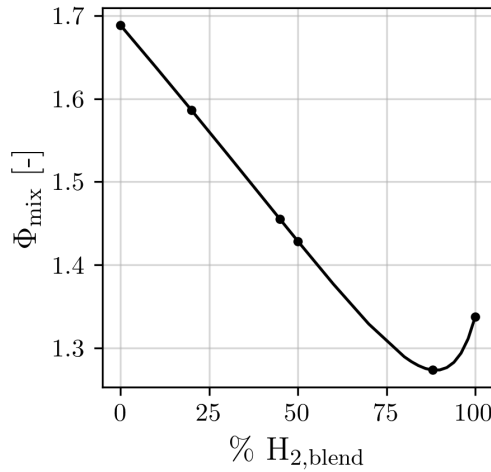


Fig. 4: Equivalence ratio of the CH_4/H_2 blend in air for conditions of Table 1 and $PA = 20$ mm.

Table 2: Cases of practical interest

	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6
$\% \text{H}_{2,\text{blend}}$	0	20	45	50	88	100
Φ_{mix}	1.68	1.58	1.45	1.42	1.27	1.33

3.1 Cases of practical interest

Figure 5 shows the $D - d$ curves for the cases listed in Table 2, and initial pressure and temperature of $p_0 = 100$ kPa and $T_0 = 300$ K. The maximum value of D for each condition corresponds to the CJ velocity, which is the ideal detonation velocity for a given initial pressure, temperature, and mixture composition. Due to heat and friction losses to the tube walls, a velocity deficit is observed as the tube diameter is decreased. All cases exhibit a turning point which indicate the minimum diameter capable of sustaining steady detonation propagation; d_{min} is thus the variable of interest in the present work. Detonation velocities at the turning point are much higher $D(d_{\text{min}}) = 1935$ m/s for case 6 ($\% \text{H}_{2,\text{blend}} = 100$, $\Phi_{\text{mix}} = 1.33$) than for case 1 ($\% \text{H}_{2,\text{blend}} = 0$, $\Phi_{\text{mix}} = 1.68$) where $D(d_{\text{min}}) = 1701$ m/s. Case 4 ($\% \text{H}_{2,\text{blend}} = 50$, $\Phi_{\text{mix}} = 1.42$) yields the lowest propagation velocity $D(d_{\text{min}}) = 1670$ m/s.

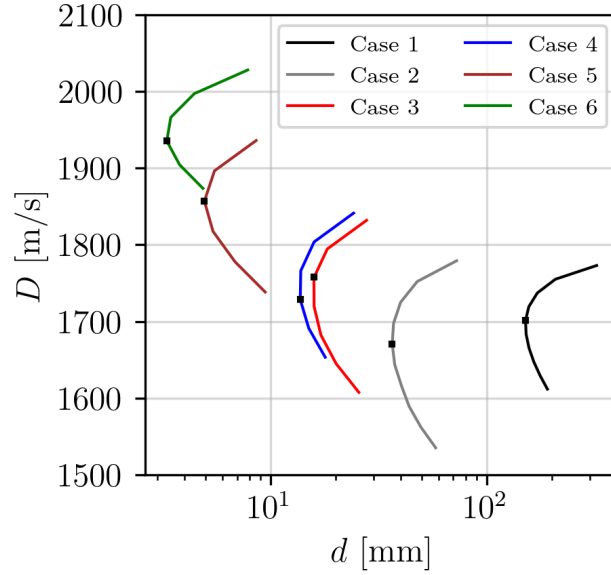


Fig. 5: $D - d$ curves for the cases of study presented in Table 2. Case 1: $\% H_{2,blend} = 0$, $\Phi_{mix} = 1.68$; case 2: $\% H_{2,blend} = 20$, $\Phi_{mix} = 1.58$; case 3: $\% H_{2,blend} = 45$, $\Phi_{mix} = 1.45$; case 4: $\% H_{2,blend} = 50$, $\Phi_{mix} = 1.42$; case 5: $\% H_{2,blend} = 88$, $\Phi_{mix} = 1.27$; case 6: $\% H_{2,blend} = 100$, $\Phi_{mix} = 1.33$.

Figure 6 summarizes our results. d_{min} decreases with increasing $\% H_{2,blend}$ content ranging from $d_{min} = 151.3$ mm ($\% H_{2,blend} = 0$) to $d_{min} = 3.3$ mm ($\% H_{2,blend} = 100$). Comparing d_{min} values with the mixing tube diameter, d_{mixer} , of a conventional NG burner, cases 3 to 6 do not meet the safety criterion since $d_{min} < d_{mixer}$. While the model predicts that a fuel blend with $\% H_{2,blend} < 45$ would not in principle require a redesign of current NG burners, the risk of flashback and propagation of fast flames in the mixing tube remains because the fuel blends are always below the UFL_{blend} (see Figure 2).

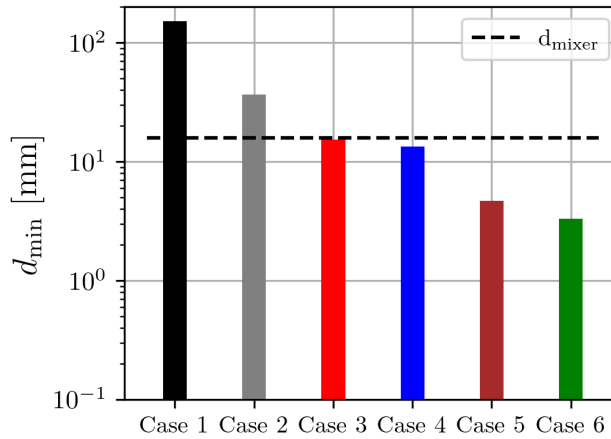


Fig. 6: Summary of d_{min} obtained for the cases of study presented in Table 2. Case 1: $\% H_{2,blend} = 0$, $\Phi_{mix} = 1.68$; case 2: $\% H_{2,blend} = 20$, $\Phi_{mix} = 1.58$; case 3: $\% H_{2,blend} = 45$, $\Phi_{mix} = 1.45$; case 4: $\% H_{2,blend} = 50$, $\Phi_{mix} = 1.42$; case 5: $\% H_{2,blend} = 88$, $\Phi_{mix} = 1.27$; case 6: $\% H_{2,blend} = 100$, $\Phi_{mix} = 1.33$. The horizontal dashed line is a visual indicator showing the mixer diameter, d_{mixer} , of a typical NG cooktop burner.

Initial temperature (T_0) variations were also examined to evaluate seasonal changes, i.e., winter (0° C), summer (25° C), and standard conditions (15° C). d_{min} exhibits a very weak dependence on T_0 (not shown here).

Note that the results presented in this section do not allow to determine the sensitivity of d_{\min} to individual changes in $\% \text{H}_{2,\text{blend}}$, and Φ_{mix} , since leaving the burner operating parameters constant, both variables change simultaneously; subsection 3.2 addresses this issue.

3.2 Effect of Φ_{mix} and $\% \text{H}_{2,\text{blend}}$ on d_{\min}

Figure 7 (a)-(d) present the detonation velocity - tube diameter, $D - d$, curves for increasing values of equivalence ratio of the mixture, Φ_{mix} , –from stoichiometric to rich– and different levels of H_2 addition to the fuel blend, $\% \text{H}_{2,\text{blend}}$. For all Φ_{mix} analyzed, the detonation velocity dependence on decreasing $\% \text{H}_{2,\text{blend}}$ at the critical point is non-linear. The detonation velocity evaluated at the minimum diameter, $D(d_{\min})$, is highest for $\% \text{H}_{2,\text{blend}} = 100$ ($D(d_{\min}) = 1881$ m/s for $\Phi_{\text{mix}} = 1$) and lowest for $\% \text{H}_{2,\text{blend}} = 20$ ($D(d_{\min}) = 1667$ m/s for $\Phi_{\text{mix}} = 1$). It recovers higher values at $\% \text{H}_{2,\text{blend}} = 0$ ($D(d_{\min}) = 1722$ m/s for $\Phi_{\text{mix}} = 1$). The behavior just described seems to be less pronounced for richest mixture considered, i.e., $\Phi_{\text{mix}} = 1.68$.

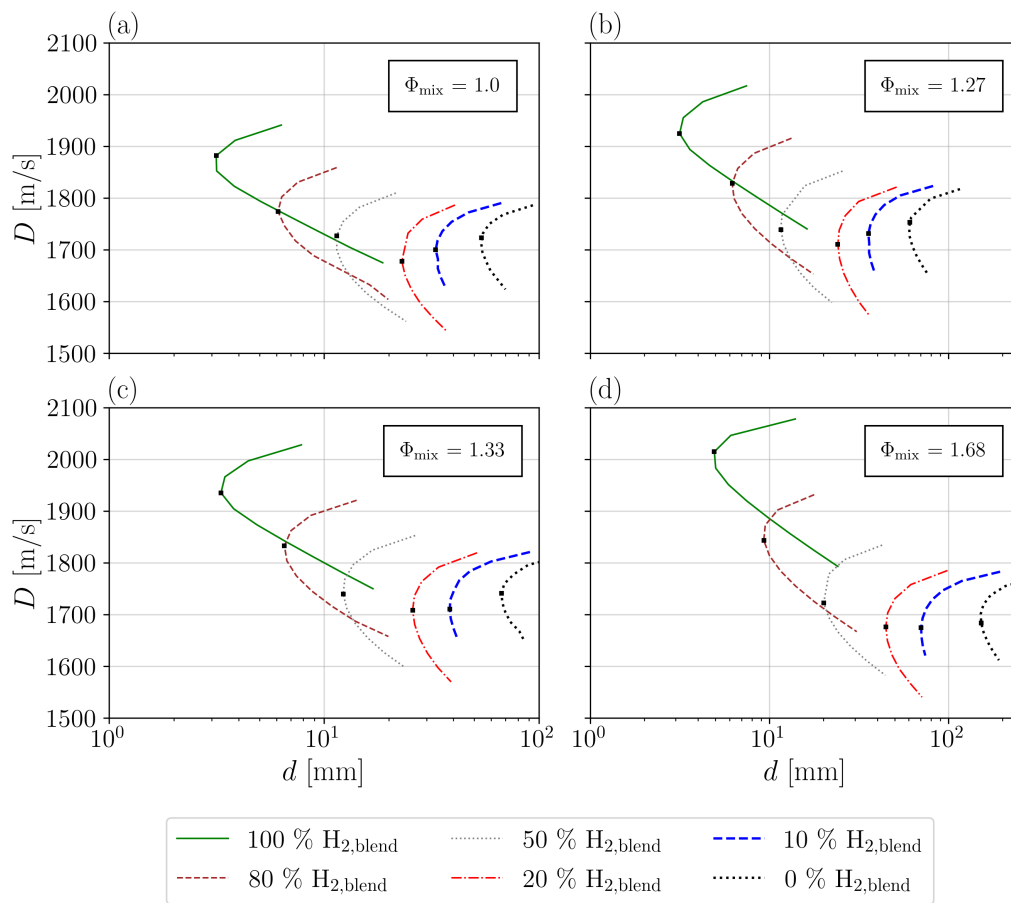


Fig. 7: $D - d$ curves for (a) $\Phi_{\text{mix}} = 1.0$, (b) $\Phi_{\text{mix}} = 1.27$, (c) $\Phi_{\text{mix}} = 1.33$, and (d) $\Phi_{\text{mix}} = 1.68$.

Figure 8 summarizes the d_{\min} values for the conditions evaluated. For all Φ_{mix} , a decrease in d_{\min} is obtained as $\% \text{H}_{2,\text{blend}}$ increases. d_{\min} shows a modest dependence on equivalence ratio for $1.0 \leq \Phi_{\text{mix}} \leq 1.33$ and decreases as $\Phi_{\text{mix}} \rightarrow 1.0$. Also, the effect of Φ_{mix} on d_{\min} is less pronounced for increasing $\% \text{H}_{2,\text{blend}}$.

Finally, to relate our results with the cellular structure of detonations, an empirical figure of merit for detonation limits in tubes can be used in which the arc length, πd_{\min} , is compared with experimental cell sizes, λ . Since there seems to be no data available for CH_4/H_2 blends at the stoichiometry and initial pressure considered, the comparison is carried out for stoichiometric H_2 -air ($\lambda = 8.18$ mm (Ciccarelli et al., 1994)) and CH_4 -air ($\lambda = 349.53$ mm (Beeson et al., 1991)). πd_{\min} for the former

mixture is 9.17 mm ($\lambda/\pi d_{\min} = 0.89$) whereas for the latter is 167.60 mm ($\lambda/\pi d_{\min} = 2.08$). These ratios suggest that the model predictions provide reasonable values, taking into account that the cellular structures of the fuel-air mixtures are irregular, and the measured cell sizes can easily vary by a factor of two among different groups (Kaneshige and Shepherd, 1997).

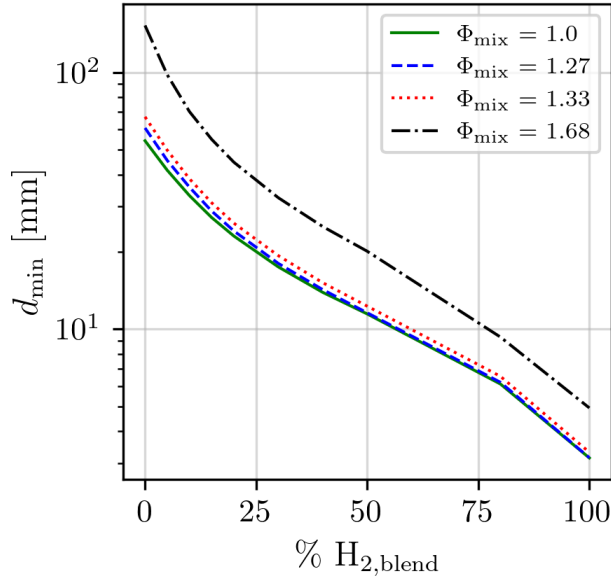


Fig. 8: Summary of d_{\min} for different Φ_{mix} values for different CH_4/H_2 blendings.

4 Conclusions

The minimum diameters, d_{\min} , for different CH_4/H_2 fuel blends in air were determined using a one-dimensional model including friction and heat losses. Operating conditions relevant to a conventional NG burner were considered. The main learnings are:

- Keeping the operating parameters of a NG burner (i.e., injection pressure, discharge coefficient, injector diameter, and primary air regulator opening) constant: (i) the equivalence ratio of the mixture, Φ_{mix} , in the mixing tube decreases with increasing % $\text{H}_{2,\text{blend}}$, going from 1.68 for 0 % $\text{H}_{2,\text{blend}}$ to 1.27 for 88 % $\text{H}_{2,\text{blend}}$, at which point, Φ_{mix} increases to 1.33 for 100 % $\text{H}_{2,\text{blend}}$. All these mixtures lie below the UFL posing a potential ignition and flame propagation hazard inside the mixing tube that can potentially result in a detonation. (ii) For blends with % $\text{H}_{2,\text{blend}} > 45$, the mixing tube diameter, d_{mixer} , is greater than d_{\min} . This suggests that NG cooktops burners may need to be redesigned to work with CH_4/H_2 blends with high H_2 content. This has strong implications in achieving the final goal of a full transition to H_2 as all appliances in the residential/industrial sector may need to be replaced or retrofitted. Strong government-backed programs will need to be put in place.
- As the $\text{H}_{2,\text{blend}}$ concentration increases, a considerable decrease in d_{\min} for all Φ_{mix} evaluated was observed. Smaller mixing tubes are thus required to avoid potential ignition, flame propagation and detonation hazards when replacing NG with CH_4/H_2 blends.
- As $\Phi_{\text{mix}} \rightarrow 1.0$, d_{\min} decreases for all the CH_4/H_2 blends evaluated. As the % $\text{H}_{2,\text{blend}}$ content increases, the effect of Φ_{mix} on d_{\min} is weaker.

Future work will investigate the influence of the actual composition of NG (C_2H_6 , C_3H_8 , C_4H_{10} , N_2 , CO_2 , etc) on the minimum tube diameters predicted by our model.

Acknowledgements

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5 Appendix A

Figure 9 (a), (b) and (c) show a comparison between numerical and experimental data available in the literature for CH₄-O₂, H₂-O₂, and H₂-air mixtures, respectively; the ratio $d_{\min,\text{num}}/d_{\min,\text{exp}}$ is also presented.

For CH₄-O₂, good predictions are obtained in the range $0.33 < \Phi < 1.2$, whereas considerable deviations are present for $\Phi > 1.2$. Note that the experimental data for this mixture is quite dated (Pusch and Wagner, 1962), and the authors did not report error bars with their results.

For H₂-O₂, the agreement between experiments and model predictions is good in the range $0.15 < \Phi < 3.6$. Leaner mixtures ($0.1 < \Phi < 0.15$) exhibit large deviations. Note that $\Phi = 0.1$ is very close to the lower flammability limit of H₂-O₂.

For H₂-air, all data points within the range $0.8 < \Phi < 2.5$ show $d_{\min,\text{num}}/d_{\min,\text{exp}}$ ratios close to unity, but deviations exist for ultra-lean mixtures. Analogous to the experimental data for CH₄-O₂, the experiments reported by Agafonov and Frolov in 1994 do not include error bars.

The over predictions for H₂-O₂/air at ultra-lean conditions are somewhat not surprising since detailed kinetic models tend to be less reliable in these regions.

The validation exercise performed shows that the 1-D model is in agreement with experimental data as $\Phi \rightarrow 1.0$, which is the most stringent condition for detonation limits as shown in Figure 8 of the manuscript; this data point could thus serve as a target for future design of cooktop burners. While the model seems to provide acceptable results for safety engineering purposes, further validation against binary fuel mixtures (CH₄/H₂) is required when new experimental data becomes available.

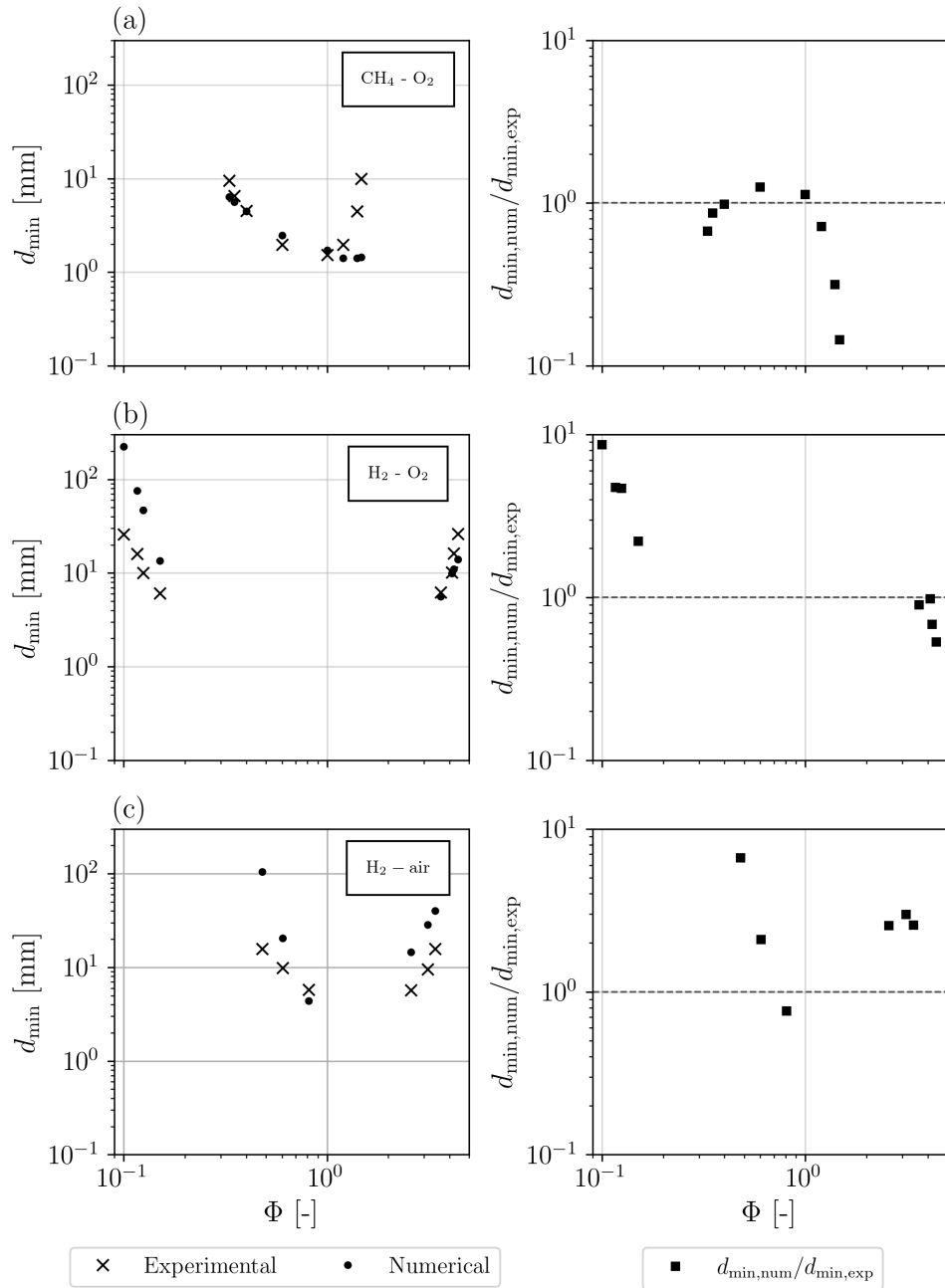


Fig. 9: Comparison between numerical and experimental results for the mixtures (a) CH₄-O₂ (Pusch and Wagner, 1962) (for $\Phi = 1.0$ Gao et al. (2014)), (b) H₂-O₂ (Agafonov and Frolov, 1994) and (c) H₂-air (Agafonov and Frolov, 1994).