Detonation cell sizes in hydrogen-methane blends

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1 Introduction

Hydrogen–methane gas blends are receiving increasing attention as an intermediate low-carbon fuel to decarbonize our energy systems and transition to a hydrogen economy. There have been a number of studies demonstrating the use of methane-hydrogen mixtures, for example, in internal combustion engines (ICE) [1] and other engineering systems such as domestic boilers [2, 3] to improve combustion efficiency and emission characteristics.

Several fundamental combustion studies have been carried out on the hydrogen-enriched methane fuel such as ignition delay time [4] and laminar burning velocity [5, 6]. Adding hydrogen to methane not only increases the combustion rate and flame speed, as well as widen the flammability limit, but the use of such a hydrogen-containing fuel also leads to safety concerns for storage and transportation due to its propensity for explosion and detonation and risks of abnormal combustion in ICE. Some studies have been conducted on the explosion characteristics of hydrogen-methane mixtures [7, 8]. Relatively little detonation data such as cell size has been reported in the literature which is of importance for safety assessment and hazard prevention [9].

Therefore, in this study, smoked-foil experimental data are gathered along with predictions from our recently developed DNN model [10, 11] to report a new set of cell size data on H_2/methane blend mixtures. This comes as a preliminary step to assess their detonation hazards and future scaling with other detonation dynamic parameters. The cell size data and detonation sensitivity of the mixtures are complemented with the induction length analysis.

2 Experimental data

For hydrogen-methane fuel-oxygen mixtures, the stoichiometric balance equation is:

$$\alpha \cdot H_2 + (1-\alpha) \cdot CH_4 + \beta \cdot O_2 \rightleftharpoons a \cdot CO_2 + b \cdot H_2O$$

with $a = (1-\alpha)$, $b = (2-\alpha)$ and $\beta = 2-3/2\alpha$ where α is the vol. % of H_2 in the blend fuel. Experimental cell size measurements in three stoichiometric hydrogen-methane blends (i.e., α = 66%, 50% and 80%) were already reported in [12], obtained using a 1.2-m long, 68 mm inner diameter steel driver section followed

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by a test section of tube with 2.5 m in length and an inner diameter of 36 mm. Additional cell size measurements for different hydrogen content (0%, 25%, 75%, 100%) in the fuel blend and initial sub-atmospheric pressure are being obtained from the detonation tube facility at Shanghai Jiao Tong University with a square cross-section of 38.1 mm by 63.5 mm and a length of 2.5 m [13], using the standard smoked foil technique and also open-shutter photography method for long exposure to capture cell sizes, as illustrated in Fig. 1.

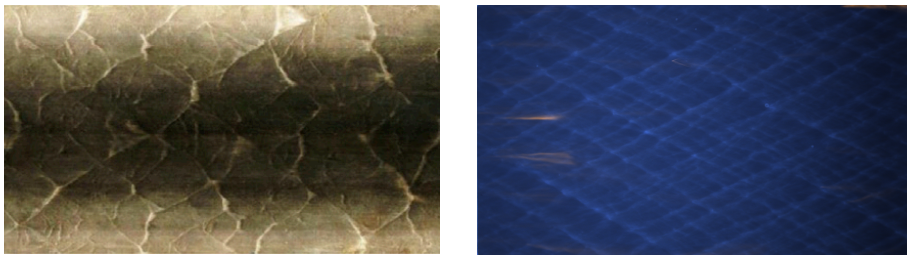

Figure 1: Cell size measurement using both the standard smoked foil technique [12] and open-shutter photography

3 Prediction using our Deep Neural Network (DNN) model

In this work, we used an improved version of our recently developed Deep Neural Network (DNN) model [10, 11] to predict the cell size in hydrogen-methane blends. This model was created using experimental cell size data for various reactants and initial conditions, for a total of 490 data points, and requires as inputs only ZND parameters that are obtained from thermodynamic equilibrium and chemical kinetics calculations. In this work, these were calculated using the CHEMKIN II package [14] with Konnov's v.0.4 detailed reaction mechanism [15]. This specific DNN model, seen in Figure 3, requires as inputs 4 non-dimensional parameters (M_{CJ}, $\dot{\sigma}^*_{max}$, ε_I, γ), where M_{CJ} is the C-J Mach number, $\dot{\sigma}^*_{max}$ is the non-dimensional thermicity that is obtained using the induction length and the speed of sound in the reactants ($\dot{\sigma}^*_{max} = \dot{\sigma}_{max} \cdot \Delta_I / c_0$), ε_I the activation energy of the induction period and γ the ratio of specific heats in the reactants. Compared to the first version of the model, the current one uses only non-dimensional inputs and prediction target (λ/Δ_I), leading to improved model predictions. The model structure has been supplemented with dropout layers, which improve the training process of the model and lead to a better determination of the uncertainty in the model's predictions. The dropout ratio has been set as 0.1 for all dropout layers, which are placed after each one of the hidden layers. In this model, there are 4 hidden layers, with 476, 248, 109 and 55 nodes for each hidden layer.

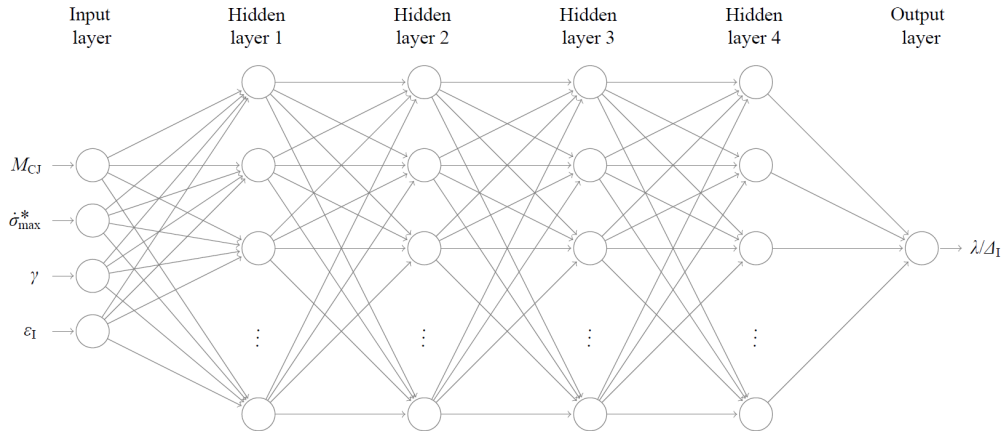

Figure 2: Deep Neural Network structure

4 Results

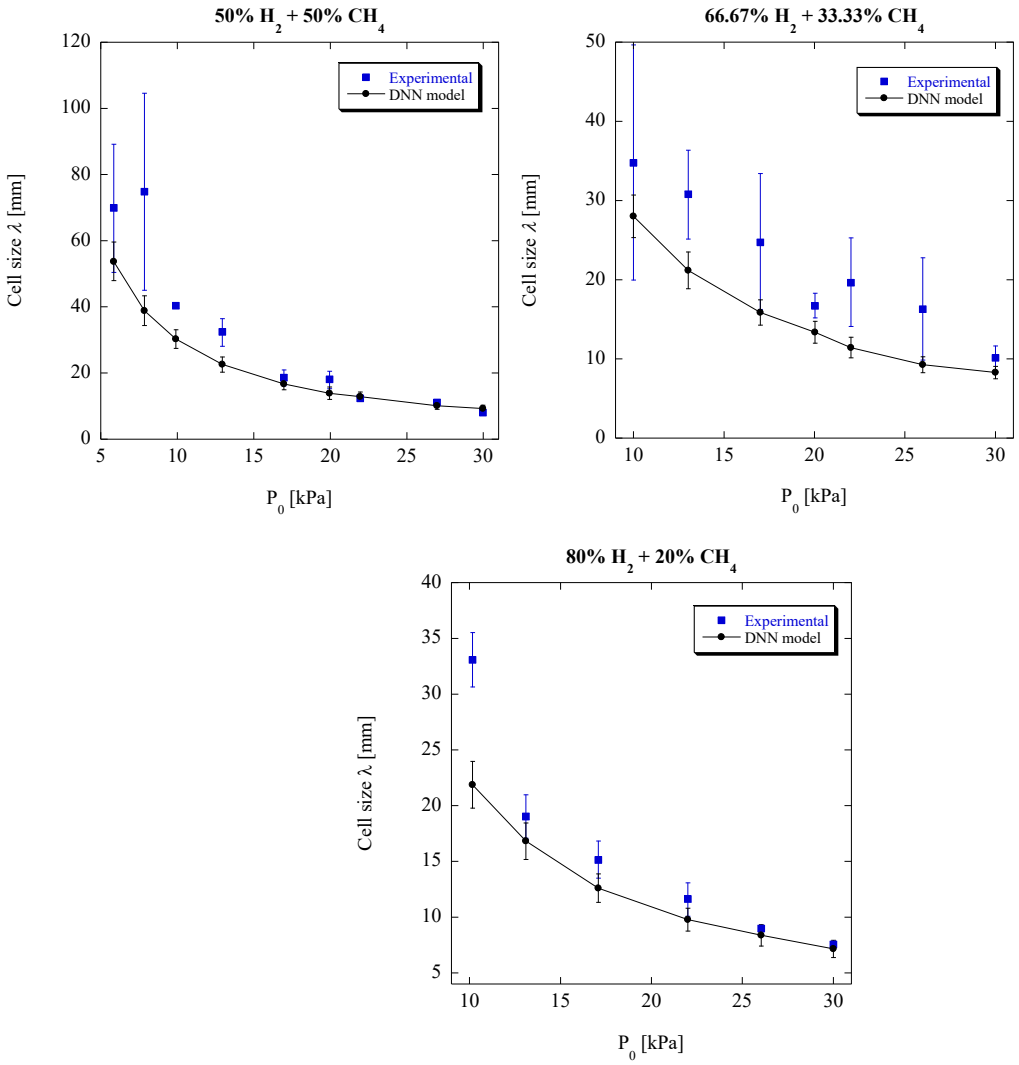

Figure 3: Cell size variation with initial pressure for three vol. % of H_2 cases in the hydrogen-methane-oxygen blends.

Figure 3 shows the comparison between the experimental measurement and the DNN prediction for three stoichiometric mixtures with different fuel compositions. For the DNN prediction, the accuracy is within 48.1% with an average of 22.2%. The DNN model appears to under-predict the cell size compared to the experimental data, especially when the initial pressure decreases and approaches the detonation limit, at which the cell size becomes comparable to the tube's dimension and is being affected by the boundary. In Figure 4 that follows, the prediction of cell size variation with initial pressure for different vol. % of H_2 is presented and will be compared with additional experimental data for further validation of the DNN model.

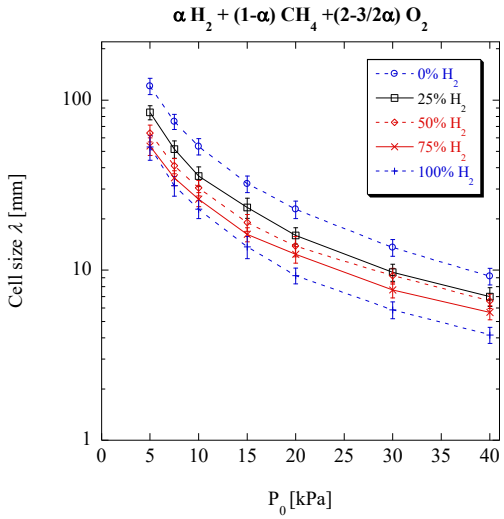

Figure 4: Cell size variation as a function of initial pressure with different vol. % of H_2 in hydrogen-methane-oxygen blend mixtures

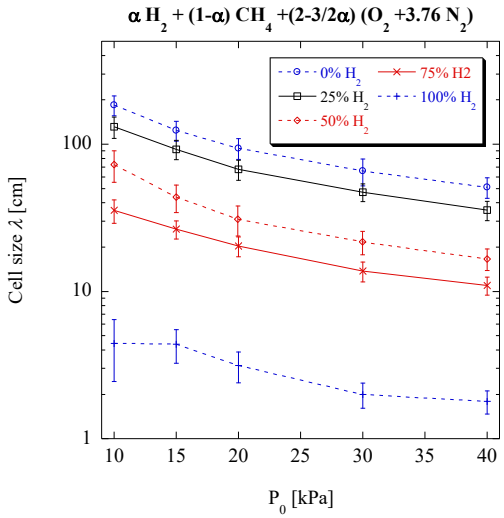

Figure 5: Cell size variation as a function of initial pressure with different vol. % of H_2 in hydrogen-methane-air blend mixtures

Using the DNN predictive tool, we also estimate the detonation characteristic cell size for the blend fuel-air mixtures: $\alpha{\cdot}H_2 + (1\text{-}\alpha){\cdot}CH_4 + \beta{\cdot}(O_2 + 3.76\ N_2) \rightleftharpoons \alpha{\cdot}CO_2 + b{\cdot}H_2O + 3.76\beta{\cdot}\ N_2$. These results are shown in Fig. 5. The higher H_2 in the fuel composition can significantly reduce the characteristic detonation cell size, prompting the blend mixture to be more detonation sensitive.

5 Concluding remarks

In the ongoing energy transition, hydrogen-enriched methane fuel represents an intermediate low-carbon step towards decarbonization and energy efficiency improvement. This study re-examines the potential impact of this blend fuel by assessing its detonation sensitivity through the measurement and prediction of characteristic detonation cell size. The use of DNN for the cell size prediction provides a quick and efficient way to obtain this dynamic parameter. From this study, some adjustments could be proposed

to further improve the prediction accuracy of the DNN model. The model's evaluation criteria could be modified for the training and testing stages in order to better account for outliers or data errors. Additional ML techniques could also be implemented to improve the model, such as the k-fold cross validation or model ensembling, as well as the addition of more experimental data to train the model.

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