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# Large-eddy simulation of lean hydrogen–methane turbulent premixed flames in the methane-dominated regime

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ABSTRACT

The application of large-eddy simulation (LES) to the prediction of $H_2$-enriched lean methane–air turbulent premixed combustion is considered. A presumed conditional moment (PCM) subfilter-scale combustion model is coupled with the flame prolongation of intrinsic low-dimensional manifold (FPI) chemistry tabulation technique. The LES and PCM-FPI modelling procedures are then applied to the prediction of laboratory-scale axisymmetric Bunsen-type turbulent premixed flames. Both premixed methane–air and $H_2$-enriched methane–air flames are considered and the predicted solutions are examined and compared to available experimental data. The enriched flame has 20% $H_2$ in terms of mole fraction and lies in the methane-dominated regime of hydrogen–methane mixtures. The LES simulations predict similar qualitative trends to those found in the experiments for flame height and curvature. The addition of $H_2$ decreases the flame height and broadens the curvature probability density functions, which show a Gaussian-type shape centred around zero. Moreover, the enriched flame displays a higher degree of wrinkling with sharper ridges of negative curvature and larger pockets of positive curvature. Overall, the proposed treatment for the PCM-FPI combustion model, in terms of progress variable and tabulated data, seems to perform well for the $H_2$-enriched methane flame in the methane-dominated regime.



## 1. Introduction

Despite the widely-recognized potential of $H_2$ as a cleaner and sustainable source of energy, the approaches for the transition from a fossil-based to hydrogen-based economy are still under discussion and the implementation of the hydrogen-based economy is expected to take decades [1,2]. Muradov and Veziroğlu [2] have extensively reviewed such transition, highlighting carbon-neutral technologies and processes (see, e.g., Ref. [3]).

$H_2$ and hydrocarbon fuel blends appear to be a promising option to synergistically pave the way toward pure hydrogen-based combustion systems while alleviating green-house gas and pollutant emissions related to fossil fuel combustion. The possibility of using hydrogen-enriched hydrocarbon fuels as a

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means for enabling greater stability of lean premixed flames with significantly reduced emissions of nitrogen oxides is also very appealing.

While promising, the wide-spread application of hydrogen-enriched hydrocarbon fuels in practical premixed combustion devices has been limited by an incomplete understanding of hydrogen-enriched combustion. In particular, the current understanding, in terms of theoretical and computational models, is unable to fully explain the experimental observations for such flames.

A number of previous studies have been conducted on the performance and emission characteristics of practical devices using $H_2$-enriched hydrocarbon fuels [4–7]. It has been found that hydrogen enrichment extends the lean stability limit and decreases emissions of carbon monoxide (CO), nitrogen oxides ($NO_x$), and unburned hydrocarbons (UHC) in spark-ignition engines, power-generation gas turbines, and aircraft gas turbines. There have also been several studies focused on fundamental aspects of hydrogen–hydrocarbon flames. It has been reported that $H_2$-enriched flames display higher laminar flame speeds, extended lean flammability limits, and augmented resistance to strain [8–12]. Moreover, experiments in swirl-stabilized burners [13,14] have been conducted to investigate the stabilization and blowout characteristics of $H_2$-enriched methane–air premixed flames. It has also been shown that the addition of $H_2$ to methane ($CH_4$) extends the flame lean stability limit, allowing stable burner operation at lower flame temperatures and reducing $NO_x$ emissions. Of particular note to the present work, Di Sarli and Di Benedetto [15] have identified three regimes of laminar burning velocity in terms of the mole fraction of $H_2$ in the fuel, $\varkappa(\varkappa = n_{H_2}/(n_{H_2} + n_{CH_4}))$. They are: (i) the methane-dominated combustion regime $(0 < \varkappa < 0.5)$; (ii) the transition regime $(0.5 \leq \varkappa \leq 0.9)$; and (iii) the methane-inhibited hydrogen combustion regime $(0.9 < \varkappa < 1)$. Numerical treatment for the so-called "methane-dominated regime" is the primary focus here.

There have been only a few previous computational studies of multi-dimensional $H_2$-enriched methane–air turbulent premixed flames. Hawkes and Chen [16] performed two-dimensional (2D) direct numerical simulations (DNS) of freely propagating flames in decaying turbulence with complex reduced chemistry (15-step reaction mechanism). Dunstan and Jenkins [17] simulated 2D premixed kernels in decaying turbulence using DNS with detailed chemistry. Day et al. [18] performed a 2D study to characterize lean methane–air flames with significant hydrogen addition, including detailed transport and chemical kinetics. Finally, Vreman et al. [19] carried out three-dimensional DNS of slot Bunsen flames with tabulated chemistry. In all the DNS simulations cited above, complex chemistry and preferential diffusion were taken into account and their relevance to characterize the flame behaviour were recognized.

This study considers the application of large-eddy simulation (LES) and appropriate subfilter-scale (SFS) modelling to the prediction of $H_2$-enriched lean methane–air turbulent premixed combustion. In particular, a presumed conditional moment (PCM) SFS combustion model [20] is coupled with the flame prolongation of intrinsic low-dimensional manifold (FPI) chemistry tabulation technique [21]. The LES and PCM-FPI modelling procedures are then applied to the prediction of laboratory-scale axisymmetric Bunsen-type turbulent premixed flames. Both premixed methane–air and $H_2$-enriched methane–air flames are considered and the predicted solutions are examined and compared to measured data from the experimental study of Halter et al. [22]. The enriched flame has 20% $H_2$ by volume and lies in the methane-dominated regime as defined by Di Sarli and Di Benedetto [15]. The turbulence intensity for both flames was relatively low and they are expected to correspond to the classical flamelet regime. The capability of the LES model to predict the observed behaviour is examined for this range of turbulent reactive flows.

## 2. Large-eddy simulation of turbulent premixed flames

The LES framework developed by Hernández-Pérez et al. [23,24] is used for performing this study. The framework is now briefly summarized, along with the PCM-FPI combustion model.

### 2.1. Favre-filtered governing equations

For the LES computations considered here, the Favre-filtered form of the Navier–Stokes equations governing compressible flows of a thermally perfect reactive gaseous mixture of $N$ species, neglecting Dufour, Soret and radiation effects, is used to describe the turbulent premixed combustion processes. Relevant flow parameters, $\varphi$, are either filtered using a low-pass spatial filtering procedure or Favre-filtered using a mass-weighted filter to yield $\overline{\varphi}$ or $\tilde{\varphi}$, respectively. The resulting equations are given by

$$\frac{\partial(\overline{\rho})}{\partial t} + \frac{\partial(\overline{\rho}\tilde{u}_i)}{\partial x_i} = 0, \tag{1}$$

$$\frac{\partial(\overline{\rho}\tilde{u}_i)}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{\rho}\tilde{u}_i\tilde{u}_j + \delta_{ij}\overline{p} - \check{\tau}_{ij}\right) = \overline{\rho}g_i + A_1, \tag{2}$$

$$\frac{\partial(\overline{\rho}\tilde{E})}{\partial t} + \frac{\partial}{\partial x_i}\left[\left(\overline{\rho}\tilde{E} + \overline{p}\right)\tilde{u}_i + \dot{q}_i\right] - \frac{\partial}{\partial x_j}\left(\check{\tau}_{ij}\tilde{u}_i\right) = \overline{\rho}g_i\tilde{u}_i + B_1 + B_2 + B_3, \tag{3}$$

$$\frac{\partial(\overline{\rho}\tilde{Y}_k)}{\partial t} + \frac{\partial(\overline{\rho}\tilde{Y}_k\tilde{u}_i)}{\partial x_i} + \frac{\partial\mathcal{J}_{k,i}}{\partial x_i} = \overline{\dot{\omega}}_k + C_1, \tag{4}$$

where $\overline{\rho}$ is the filtered mixture density, $\tilde{u}_i$ is the Favre-filtered mixture velocity, $\overline{p}$ is the filtered mixture pressure, $\tilde{Y}_k$ is the Favre-filtered mass fraction of species $k$, $\tilde{E}$ is the Favre-filtered total mixture energy (including chemical energy) given by $\tilde{E} = \sum_{k=1}^{N}\tilde{Y}_k(\check{h}_k + \Delta h^0_{f,k}) - \overline{p}/\overline{\rho} + \widetilde{u_i u_i}/2$; $\check{h}_k$, $\Delta h^0_{f,k}$ and $\overline{\dot{\omega}}_k$ are the sensible enthalpy (evaluated in terms of the Favre-filtered temperature), heat of formation and the filtered reaction rate of species $k$, respectively, and $g_i$ is the acceleration due to gravity. The filtered equation of state adopts the form $\overline{p} = \overline{\rho}R\tilde{T}$, assuming that the SFS temperature-species correlation is negligible. Here, $\tilde{T}$ is the Favre-filtered mixture temperature and $R$ is the gas constant. The resolved stress tensor, $\check{\tau}_{ij}$, the