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Turbulence-chemistry interaction in lean premixed hydrogen combustion

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Abstract

This paper presents three-dimensional direct numerical simulations of lean premixed hydrogen flames at an equivalence ratio of $\varphi = 0.4$ over a range of turbulence levels from Ka = 1–36. The simulations form part of a larger effort to construct a DNS database that can be used by the community for model construction and validation. We have focussed on producing well-resolved simulations at conditions representative of atmospheric laboratory-scale flames. After an overview of phenomenological trends with increasing Karlovitz number, we examine the factors that lead to an observed decorrelation between fuel consumption and heat release in the flame at Ka = 36. We show that in this flame the fuel consumption is greatly enhanced in regions of positive curvature. We also show that the radical pool is enriched throughout the entire flame as Ka is increased. In particular, we identify three reactions that, driven by high molar concentrations of radicals at low temperatures, are responsible for high levels of heat release away from regions of fuel consumption, thereby accounting for the observed decorrelation between fuel consumption and heat release.

Keywords: Turbulent combustion; Premixed hydrogen flames; Low Mach number combustion

1. Introduction

There has been considerable recent interest in hydrogen or hydrogen-rich mixtures obtained from gasification of coal or biomass. These types of fuels provide clean alternatives to traditional petroleum and natural gas fuels. Burning under lean conditions reduces the exhaust gas temperatures, and consequently, thermal NO_x emissions.

At low-to-moderate levels of turbulence, the thermodiffusive instability leads to flames that burn in well-known cellular structures, which results in localised hot spots where the flame is burning more intensely due to local enrichment of fuel by diffusion [1–6]. At high turbulence levels, hydrogen flames transition to the distributed burning regime where the thermodiffusive instability is dominated by turbulent mixing [7,8].

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In the present paper, we present simulations of lean premixed hydrogen over a range of low-to-moderate turbulence levels. The simulations form part of a larger effort to construct a DNS database that can be used by the community for model construction and validation. We have focussed on producing well-resolved simulations with conditions that are representative of atmospheric laboratory-scale flames, rather than the more highly turbulent conditions of distributed flames.

We consider lean premixed hydrogen flames at an equivalence ratio $\varphi = 0.4$. The characterisation of the turbulence in terms of the flame structure is given by the Karlovitz and Damköhler numbers. In Aspden et al. [9], we note that a freely-propagating lean hydrogen flame is distinctly different from the idealised flat laminar flame because of the thermodiffusive instability. We showed that a flame speed and thickness defined from a freely-propagating flame provide a better normalisation of flame behaviour than the laminar values. Thus, following [9] we work with freely-propagating Karlovitz and Damköhler numbers, defined as

$$\mathrm{Ka}^2 = \frac{\breve{u}^3}{s_F^3}\frac{l_F}{l} \quad \text{and} \quad \mathrm{Da} = \frac{s_F}{\breve{u}}\frac{l}{l_F}, \tag{1}$$

respectively, where $\breve{u}$ and l are the turbulent rms velocity and integral length scale, respectively, and s_F and l_F are the freely-propagating flame speed and width, respectively.

For the present simulations, we consider an idealised configuration with a fixed domain width and integral length scale. Turbulence in the fluid is driven via a time-dependent zero-mean volumetric fluid forcing term [8,10]. The resulting turbulence intensity is controlled by adjusting the amplitude of the forcing.

We briefly sketch the computational methodology and describe the present study in Section 2. In Section 3 we present the results of the simulations, starting with an overview of the observations and trends with Karlovitz number in Section 3.1, and the identification of an interesting decorrelation between fuel consumption and heat release, which is explored further in Section 3.2. We then examine the individual reactions that contribute to this decorrelation in Section 3.3, and conclude with an interpretation of the results in Section 4.

2. Computational methodology

The simulations presented here are based on a low Mach number formulation of the reacting flow equations. The methodology treats the fluid as a mixture of perfect gases. We use a mixture-averaged model for differential species diffusion and ignore Soret, Dufour, gravity and radiative transport processes. With these assumptions, the low Mach number equations for an open domain are

$$\frac{\partial(\rho \boldsymbol{u})}{\partial t} + \nabla\cdot(\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla\pi + \nabla\cdot\tau + \rho\boldsymbol{F},$$
$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla\cdot(\rho Y_i \boldsymbol{u}) = \nabla\cdot(\rho\mathcal{D}_i\nabla Y_i) - \dot{\omega}_i,$$
$$\frac{\partial(\rho h)}{\partial t} + \nabla\cdot(\rho h\boldsymbol{u}) = \nabla\cdot\left(\frac{\lambda}{c_p}\nabla h\right) + \sum_i \nabla\cdot\left[h_i\left(\rho\mathcal{D}_i - \frac{\lambda}{c_p}\right)\nabla Y_i\right],$$

where ρ is the density, $\boldsymbol{u}$ is the velocity, π is the perturbational pressure, Y_i is the mass fraction of species i, h is the mass-weighted enthalpy of the gas mixture, T is the temperature, and $\dot{\omega}_i$ is the net destruction rate for species i due to chemical reactions. Also, λ is the thermal conductivity, τ is the stress tensor, c_p is the specific heat of the mixture, and $h_i(T)$ and $\mathcal{D}_i$ are the enthalpy and mixture-averaged diffusion coefficients of species i, respectively. Here $\boldsymbol{F}$ is a long-wavelength forcing term designed to establish and maintain turbulence with the desired properties. These evolution equations are supplemented by an equation of state for a perfect gas mixture. The reader is referred to [11] for details of the low Mach number model and its numerical implementation. The chemical kinetics and transport are modelled using the Li et al. hydrogen mechanism [12], which consists of 9 species with 19 fundamental reactions.

The overall numerical scheme converges with second-order accuracy in both space and time. The performance of the scheme for direct numerical simulation of premixed flame systems in regimes comparable to the present study was examined in [10]. An *effective* Kolmogorov length scale was formulated, which measures the actual Kolmogorov length scale realised in a simulation at a given resolution. Here, the most computationally demanding simulation, having the highest turbulence levels, has a computational cell width that is approximately 0.75 times the Kolmogorov length scale. At this resolution, the numerical scheme produces an *effective* Kolmogorov length scale that is just 3% larger than the analytical value; the other simulations are better resolved. Also, the grid spacing for all cases considered is such that 25 cells span the thermal thickness of a freely-propagating flame corresponding to this fuel–air mixture; note that there are over 40 cells across the unstrained flat laminar flame. Thus, the flame and the turbulence are numerically well-resolved in all four of the cases we considered here.

2.1. Simulation configuration

We simulated four downward-propagating flames in a high aspect ratio domain (8:1), with periodic lateral boundary conditions, a free-slip base and outflow at the top. The momentum source term