Three-dimensional direct numerical simulation of turbulent lean premixed methane combustion with detailed kinetics

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ABSTRACT

The interaction of maintained homogeneous isotropic turbulence with lean premixed methane flames is investigated using direct numerical simulation with detailed chemistry. The conditions are chosen to be close to those found in atmospheric laboratory experiments. As the Karlovitz number is increased from 1 to 36, the preheat zone becomes thickened, while the reaction zone remains largely unaffected. A negative correlation of fuel consumption with mean flame surface curvature is observed. With increasing turbulence intensity, the chemical composition in the preheat zone tends towards that of an idealised unity Lewis number flame, which we argue is the onset of the transition to distributed burning, and the response of the various chemical species is shown to fall into broad classes. Smaller-scale simulations are used to isolate the specific role of species diffusion at high turbulent intensities. Diffusion of atomic hydrogen is shown to be related to the observed curvature correlations, but does not have significant consequential impact on the thickening of the preheat zone. It is also shown that susceptibility of the preheat zone to thickening by turbulence is related to the 'global' Lewis number (the Lewis number of the deficient reactant); higher global Lewis number flames tend to be more prone to thickening.

1. Introduction

Direct numerical simulation with detailed kinetics provides a powerful tool for studying the fundamentals of turbulent combustion, and for the development and validation of turbulent flame models for engineering applications. As part of the effort to develop clean-burning efficient systems to meet growing global energy demands, there is significant interest in lean premixed methane combustion. Burning under lean conditions reduces the exhaust gas temperatures, and consequently, thermal NO_x emissions. In this paper, three-dimensional direct numerical simulations of lean premixed methane combustion with detailed kinetics are presented over a range of turbulent intensities representative of the conditions found in typical experimental studies. The focus of the study is on the interactions between turbulence and combustion, and how the flame is affected as turbulent intensity increases. The goal is to provide a set of benchmark DNS data that can be used both to study basic flame physics and to provide a baseline for evaluation of turbulent combustion models.

There is a growing body of work in the literature that deals with turbulent premixed methane flames with detailed kinetics. The earliest work in this area investigated two-dimensional configurations using a detailed C1 mechanism [1–4]. Bell et al. [5] produced the first simulation of a turbulent methane flame in three dimensions with moderate-fidelity kinetics using DRM-19, which is a simplified mechanism derived from GRIMech 1.2. Simulations using DRM-19 for a variety of experimental configuration have been presented in [6,7]. Sankaran et al. [8] performed a DNS of the lean premixed preheated methane flame stabilised on a slot burner using a skeletal mechanism with 13 species derived from GRIMech 1.2. More recently, Aspden et al. [9] and Carlsson et al. [10,11] presented DNS of lean premixed methane flames at high turbulence levels near to the transition to distributed burning. The simulations presented in the present paper were conducted using GRIMech 3.0 without the emissions chemistry [12,13].

Here lean premixed methane flames are considered at an equivalence ratio of $\varphi = 0.7$, for which the Lewis number of the fuel is close to unity; the Lewis number of the fuel (i.e. the deficient reactant) will be referred to as the global Lewis number. The characterisation of the turbulence in terms of the unstrained laminar flame properties is given by the Karlovitz and Damköhler numbers,

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which are defined by

$$Ka^2 = \frac{\Upsilon^3}{\Lambda} = \frac{u^3}{s_F^3}\frac{l_F}{l} \quad \text{and} \quad Da = \frac{\Lambda}{\Upsilon} = \frac{s_F}{u}\frac{l}{l_F}$$

where u and l are the turbulent rms velocity fluctuation and integral length scale, respectively, and s_F and l_F are the unstrained flat laminar flame speed and width, respectively, $\Lambda = l/l_F$ and $\Upsilon = u/s_F$. The Damköhler number represents the ratio of chemical and integral length time scales. The Karlovitz number represents the ratio of Kolmogorov and chemical time scales, and can be thought of as a measure of the strength of the turbulence relative to the flame. From the point of view of turbulence-flame interactions, the more relevant parameter is the Karlovitz number; fixing Ka effectively fixes the energy dissipation rate $\varepsilon = u^3/l$ and the Kolmogorov length scale $\eta = (\nu^3/\varepsilon)^{1/4}$, and therefore the turbulence that interacts with the flame. In the present paper, Karlovitz numbers between 1 and 36 are presented. Turbulence is generated by incorporating a forcing term into the momentum equations that can be adjusted to match desired turbulence properties using our well-established approach [14–16]. The same domain size is used for all simulations, which results in a fixed integral length scale, approximately one-tenth the width of the domain, and four times the thermal thickness of the unstrained laminar flame (i.e. $\Lambda = 4$). The conditions that are considered are typical of those encountered in a range of atmospheric laboratory scale experiments; i.e. turbulent velocity fluctuations on the order of a few metres per second and an integral length scale on the order of a few millimetres.

The computational methodology and simulation configuration are presented in Section 2. An overview of the simulations and flame response to increasing Karlovitz number are then presented in Section 3.1, followed by joint probability density functions of flame speed and curvature in Section 3.2. Two-dimensional slices through the three-dimensional data present changes in chemical composition in Section 3.3, and thickening of the preheat zone is examined in Section 3.4. The chemical composition is explored further through conditional means of species molar concentration in Section 3.5. The effect of diffusive processes are investigated by running further small-scale simulations in Section 4, where species diffusion coefficients are artificially adjusted. In particular, several key observations are shown to be related to the high mobility of atomic hydrogen. This is demonstrated using slices (Section 4.1), joint probability density functions (Section 4.2), flame thickening (Section 4.3), and conditional means of molar concentrations (Section 4.4). The paper closes with a summary of the conclusions (Section 5).

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. A mixture-averaged model is used for differential species diffusion, ignoring Soret and Dufour effects, as well as neglecting gravity and radiative transport processes. With these assumptions, the low Mach number equations for an open domain are

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla\cdot(\rho\mathbf{u}\mathbf{u}) = -\nabla\pi + \nabla\cdot\tau + \rho\mathbf{F},$$

$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla\cdot(\rho Y_i\mathbf{u}) = \nabla\cdot(\rho\mathcal{D}_i\nabla Y_i) - \rho\dot{\omega}_i,$$

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

where ρ is the density, $\mathbf{u}$ is the velocity, Y_i is the mass fraction of species i, h is the specific 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 specific enthalpy and mixture-averaged diffusion coefficients of species i, respectively. Here, $\mathbf{F}$ 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 basic discretisation combines a symmetric operator-split treatment of chemistry and transport with a density-weighted approximate projection method. The projection method incorporates the equation of state by imposing a constraint on the velocity divergence. The resulting integration proceeds on the time scale of the velocity with advective transport treated explicitly. Faster diffusion and chemistry processes are treated time-implicitly. This integration scheme is embedded in a parallel adaptive mesh refinement algorithm framework based on a hierarchical system of rectangular grid patches. The complete integration algorithm is second-order accurate in space and time, and discretely conserves species mass and enthalpy. The reader is referred to [17] for details. The chemical kinetics and transport are modelled using the GRIMech 3.0 methane mechanism [12,13] with the nitrogen chemistry removed. The resulting mechanism consists of 35 species with 217 reactions.

The overall numerical scheme is known to converge with second-order accuracy, and the ability of the scheme to perform direct numerical simulation was examined in [14]. An effective Kolmogorov length scale was formulated, which measures the Kolmogorov length scale that actually results from a simulation at a given resolution. The main simulations presented here all have an effective Kolmogorov length scale within 0.9% of the analytical value, and so the turbulence can be considered to be sufficiently-well resolved. The narrowest intermediate chemical species have a thickness (defined using the points at half of the peak value) that is spanned by approximately six computational cells; the profiles can be well reproduced with half the resolution used here, and so the chemistry can also be considered well-resolved.

2.1. Simulation configuration

Three-dimensional simulations were conducted for four statistically-stationary downward-propagating flames in a high aspect ratio domain, with periodic lateral boundary conditions, a free-slip base and outflow at the top. The turbulent background velocity field was maintained through the source term in the momentum equations following [14]. This results in a time-dependent zero-mean turbulent velocity field. It was shown in [14] that this approach gives approximately 10 integral length scales across the domain width. The domain width is $L = 2.64$ cm, which results in an integral scale of $l \approx 2.6$ mm. An inert calculation was run to establish the turbulence at reduced expense, and the reacting flow simulation was initialised by superimposing a laminar flame solution onto the turbulent velocity field.

The unburned fuel mixture was taken to have a temperature of 298 K and standard atmospheric pressure, and the equivalence ratio was taken to be $\varphi = 0.7$, which gives a global Lewis number of approximately unity. The unstrained laminar flame speed is approximately 18.9 cm/s, and the thermal thickness, as determined by the maximum temperature gradient, is approximately 660 microns. The adiabatic flame temperature is 1842 K. At the specified resolution there are over 25 computational cells across the thermal flame thickness, which is more than sufficient to resolve the flame structure. For these conditions, the integral scale is four times the flame thickness for all of the cases. The rms velocity fluctuations were varied from approximately 1.6–17 times the unstrained laminar flame speed. Details of the four cases considered are given in Table 1, and the position of these flames on the premixed regime