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Proceedings of the Combustion Institute 36 (2017) 2005–2016

Proceedings of the Combustion Institute

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Turbulence–flame interactions in lean premixed dodecane flames

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Received 4 December 2015; accepted 15 July 2016
Available online 25 July 2016

Abstract

Turbulent lean premixed dodecane/air flames are simulated in a doubly-periodic domain using detailed kinetics and transport over a range of Karlovitz number. We observe extensive thickening of thermal profiles through the flames that increases with turbulent intensity. The high Lewis number of the flames acts to suppress wrinkling of the flame resulting in considerably lower turbulent flame speeds than is observed for lower molecular weight fuels. The impact of high Lewis number is also reflected in a negative correlation of local consumption-based flame speed with curvature. Characteristic of heavy hydrocarbons, pyrolysis of the fuel into smaller fuel fragments is separated in temperature from the primary consumption of oxygen, which peaks at a higher temperature where the fuel fragments are consumed. The resulting intermediate species are partially entrained within the cool region ahead of the flame, but the overall pyrolysis-oxidation sequence appears essentially unaffected by turbulent mixing; however, the peak rates of these reactions are dramatically reduced.

Keywords: Turbulent premixed flames; Direct numerical simulation; Detailed chemistry; Low Mach number flow; Dodecane

1. Introduction

Detailed chemical models for the combustion kinetics of real fuels (e.g., gasoline, diesel, and jet fuels) are important tools for improving the design of combustion technologies. A key issue in such systems is the effect of turbulent mixing on combustion chemistry, which can be explored using detailed numerical simulation. However, real fuels contain variable blends of thousands of hydrocarbon compounds so the use of detailed models is prohibitive. Instead the focus is on dodecane with a molecular weight representative of heavy practical fuels. In particular, lean premixed dodecane/air combustion in a turbulent environment is investigated using numerical simulations, based on a

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http://dx.doi.org/10.1016/j.proci.2016.07.068
1540-7489

reduced kinetic model. There is a growing body of work of direct numerical simulation of turbulent premixed flames with detailed chemistry and transport, mostly focussing on smaller fuel molecules, such as methane and hydrogen and syngas mixtures. The goal in this work is to highlight characteristics of the chemistry–turbulence interactions specific to the pyrolysis of large-molecule fuels, and compare the oxidation and heat release of the resulting fragments to similar scenarios involving the smaller, simpler fuels.

Aspden et al. [1–3] have considered hydrogen, methane and propane flames with detailed kinetics in moderate-to-intense turbulence. Carlsson et al. [4,5] and Tanahashi et al. [6–8] have also considered turbulent premixed hydrogen and methane flames with detailed chemistry. Little work has been done on direct numerical simulation of high molecular weight hydrocarbon fuels, particularly for high Karlovitz number premixed flames. In a sequence of papers, Savard et al. [9,10] and Lapointe et al. [11] discuss simulations of premixed heptane flames at high Karlovitz numbers with detailed chemistry and transport, building on previous work [12] based on the hydrogen simulations in [1]. The focus of these papers is on the impact of differential diffusion on flame response, even at high Karlovitz numbers; the authors note a broadening of the flame and a transition to composition versus temperature profiles characteristic of a unity Lewis number flame and a reduction in heat release and fuel consumption rates.

This paper presents simulations of lean premixed dodecane flames with detailed kinetics and transport at high Karlovitz number, targetting matching conditions to our previous work [3,13], and similar in spirit to the heptane simulations discussed above, but at moderate turbulence levels. Turbulent conditions are characterised in terms of the one-dimensional unstrained steady flame properties using the Karlovitz and Damköhler numbers, which are defined by

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

where $\breve{u}$ and l are the turbulent rms velocity fluctuation and integral length scale, respectively, and s_F and l_F are the steady unstrained flame speed and width, respectively. In the present paper, cases are constructed with Ka in the range, 1–36, following the approach detailed in [1,14]. An overview of the basic flame characteristics is first presented, followed by a discussion of the differences between the behaviour of dodecane and methane in comparable premixed turbulent flames.

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; the corresponding conservation equations for an open domain are

$$\begin{aligned}
\frac{\partial(\rho \boldsymbol{u})}{\partial t} + \nabla\cdot(\rho \boldsymbol{u}\boldsymbol{u} + \tau) &= -\nabla\pi + \rho\boldsymbol{F},\\
\frac{\partial(\rho Y_i)}{\partial t} + \nabla\cdot(\rho Y_i \boldsymbol{u} + \boldsymbol{\mathcal{F}}_i) &= \rho\dot{\omega}_i,\\
\frac{\partial(\rho h)}{\partial t} + \nabla\cdot(\rho h \boldsymbol{u} + \boldsymbol{\mathcal{Q}}) &= 0,
\end{aligned}$$

where ρ is the density, $\boldsymbol{u}$ is the velocity, h is the mass-weighted enthalpy, T is temperature. Y_i is the mass fraction and $\dot{\omega}_i$ is the molar production rate for species i. A mixture-averaged model is assumed for diffusive transport, ignoring Dufour and Soret effects; τ is the stress tensor; $\boldsymbol{\mathcal{Q}} = h_i\boldsymbol{\mathcal{F}}_i - \lambda\nabla T$ is the heat flux and $\boldsymbol{\mathcal{F}}_i = -\rho\mathcal{D}_i\nabla X_i$ is the species diffusion. The momentum source term, $\boldsymbol{F}$, is a long-wavelength forcing term designed to establish and maintain turbulence with the desired properties. The chemical kinetics and transport are modelled using the dodecane mechanism of You et al. [15], consisting of 56 species with 289 fundamental reactions. These evolution equations are supplemented by CHEMKIN-compatible databases for thermodynamic quantities. Transport properties are computed using EGLIB [16].

The basic discretisation combines a spectral deferred corrections (SDC) coupling of chemistry and transport [17] with a density-weighted approximate projection method for low Mach number flow [18]. The projection method implements a constrained evolution on the velocity field via the SDC iterations, which ensures that the update simultaneously satisfies the equation of state and discrete conservation of mass and total enthalpy. A time-explicit approach is used for advection; faster diffusion and chemistry processes are treated time-implicitly, and iteratively coupled together within the defferred corrections strategy. Since the low Mach system does not support acoustic waves, the time step size is governed by a CFL constraint based on advective transport. The integration algorithm is second-order accurate in space and time.

The performance of the numerical scheme for direct numerical simulation of premixed flame systems in regimes comparable to the present study was examined in [14]. An *effective* Kolmogorov length scale, η_{eff}, 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 1.27 times the Kolmogorov length scale, η. In this case, the numerical scheme produces $\eta_{eff}/\eta < 1.03$. All other cases were better resolved.

Downward-propagating flames were simulated in a high aspect ratio domain, with periodic lateral