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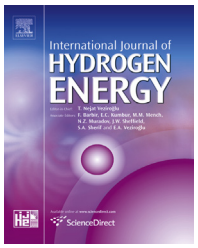

Direct numerical simulation and reaction rate modelling of premixed turbulent flames

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ABSTRACT

Direct numerical simulation (DNS) is employed to investigate the flame characteristics and the mean chemical source term $\widetilde{\omega}_k$ of hydrogen/air premixed turbulent combustion in the thin reaction zones regime. Three flames with different initial radius and equivalence ratio are considered. The probability density functions (PDFs) of the flame curvature, shape factor and turbulent flame velocity are plotted and compared for different flames. The distributions of the flame curvature and shape factor indicate that the local geometries for both of the flame kernel and planar flame are similar, irrespective of their difference in the global geometry. The modified laminar flamelet PDF (MLF-PDF) shows improvements over the widely used β-PDF for the progress variable distribution. Several closures for the conditional mean reaction rate are integrated with the presumed PDFs and compared with the DNS data. It is demonstrated that the predictions of the first-order reaction rate integrated with the MLF-PDF are satisfactory for H_2 but not for the intermediate species OH. The second-order closure integrated with the MLF-PDF is proved to be promising in predicting both of the major and intermediate species.

Introduction

The prediction of turbulent combustion is of prime importance for the design and development of combustion devices, including internal combustion engines and gas turbines. The main challenge in turbulent combustion modelling is the determination of the mean chemical source term $\widetilde{\omega}_k$. As the chemical reaction rate is usually highly nonlinear, it is difficult to express $\widetilde{\omega}_k$ as a function of the mean temperature and species mass fractions, reflecting the complexity of the turbulence–chemistry interactions. In the context of premixed combustion, many models are based on the solving of a transport equation for a reactive progress variable, while the probability density function (PDF) for the progress variable is assumed to have a specified shape. Two main categories for premixed combustion modelling include the laminar flamelet model and the conditional moment closure (CMC).

The basic idea of the laminar flamelet model is to assume that a small instantaneous flame element embedded in a turbulent flow has the structure of a laminar flame [1]. This is only truly valid in the flamelet regime in which chemistry

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time-scales are smaller than the turbulence time-scales. The laminar flamelet model is widely used in different forms in numerical simulations of premixed turbulent flames [2,3].

The CMC method was independently developed by Klimenko and Bilger [4]. It is an attractive approach for turbulent combustion modeling as it is not restricted to the flamelet regime and the predictions have been proved to be promising in many numerical simulations [5]. The CMC method was originally proposed for non-premixed combustion. Some efforts have been made to extend it for premixed combustion [6].

A number of direct numerical simulation (DNS) studies have analyzed the premixed flame structures in terms of flame tangential strain rate, curvature and so on [7–10]. However, the effects of flame configuration on the flame structures and combustion modeling are yet to be clarified. In the current work, three-dimensional DNS of two canonical configurations, i.e. the freely propagating planar flame and the spherical flame kernel, for premixed turbulent combustion with detailed chemistry is performed. The purpose is to investigate the flame structures, and the influences of the presumed PDFs and the conditional mean reaction rate closures on the prediction of the mean chemical reaction rate. The widely used β-PDF and the modified laminar flamelet PDF (MLF-PDF) proposed by Jin et al. [11] are used for the progress variable distribution. Several closures for the conditional mean reaction rate in the context of CMC/flamelet combined with the presumed PDFs are tested and compared with the DNS data *a-priori*. The remainder of the paper is organized as follows. Section 2 gives the numerical schemes. Section 3 outlines the flame configurations studied and their parameters in detail. In Section 4, the results are presented and discussed. Finally, some conclusions are drawn.

Numerical methods

The simulations are based on the solution of the fully compressible Navier–Stokes equation system for reacting flows, which are solved using a DNS code developed in our group. The spatial derivative is discretized using an eighth-order explicit central differencing scheme [12]. The time integration is carried out with the classical fourth-order explicit Runge–Kutta method. To remove spurious high frequency fluctuations in the solution, an eighth-order filter is used. More details about the DNS code can be referred to our previous paper [13].

A 9 species (H_2, O_2, O, OH, H_2O, H, HO_2, H_2O_2 and N_2) and 19-step detailed mechanism developed by Li et al. [14] for hydrogen/air combustion is used. Reverse rate constants are computed from the forward rate constants and the equilibrium constants. CHEMKIN software libraries [15,16] are linked to current code to evaluate reaction rate, thermodynamic and transport properties.

Flame configurations

Two configurations of premixed turbulent combustion are investigated using DNS. One is the freely propagating planar flame, and the other one is the spherical flame kernel. Both configurations are paramount to provide insight into turbulence–flame interactions as well as turbulent combustion model development [17]. The flame kernel is featured by its initial radius r_0. The planar flame can also be considered as a flame kernel with an infinite radius. To explore the effects of initial radius and equivalence ratio on premixed turbulent combustion, three simulations have been carried out (Table 1).

The computational domain is taken to be a cube of the size $2\pi \times 2\pi \times 2\pi$ mm^3, which is discretized using a mesh of 256^3 uniform grids, resulting in a grid spacing of 24.5 μm. For the planar flame, we initialize the flame with the corresponding unstrained laminar premixed flame profile. The temperature is 300 K and the pressure is 1.01325×10^5 Pa for the fresh gas. The laminar premixed flame is characterized by its flame velocity S_L and flame thickness δ_L, which is defined as $\delta_L = (T_2 - T_1)/(\partial T/\partial x)_{max}$, where T_2 is the temperature of the burnt gas, and T_1 is the temperature of the fresh gas. The laminar flame time scale τ_f is defined as the ratio of the laminar flame thickness to the laminar flame velocity. The flame kernels are initialized by burnt gas with an initial radius $r_0 = 0.8$ mm at the center of the computational domain, surrounded by fresh gas of hydrogen and air. In the case of planar flame, the boundaries are non-reflecting [18] in the direction of the mean flame propagation, and periodic in the lateral directions. For the spherical flame kernels, the mean flame propagates radially outward, thus, all directions are considered to be non-reflecting. In all cases, the time step is set to 1.5×10^{-8} s to satisfy the CFL (Courant–Friedrichs–Lewy) condition as well as all of the time scales for hydrogen combustion.

The initial turbulence is prescribed by a three-dimensional turbulent kinetic energy spectrum function using the pseudo-spectral method [19]. The initial values of the normalized turbulent velocity u'/S_L, the normalized integral length scale l/δ_L, the turbulent Reynolds number $Re = u'l/\nu$, where is ν the kinematic viscosity, the turbulent Karlovitz number $Ka = \tau_f/\tau_\eta$, and the turbulent Damköhler number $Da = S_L l/u'\delta_L$ are outlined. According to the regime diagram for premixed turbulent combustion proposed by Peters [20], the three cases studied are located in the thin reaction zones regime. For the purpose of comparison, the data presented in the following for the three cases are extracted at $t = 1.6\ \tau_t$, where τ_t is the eddy turned over time defined as $\tau_t = l/u'$.

Table 1 – Parameters for DNS of hydrogen/air premixed flames.

Case	ϕ	r_0(mm)	S_L(m/s)	δ_L(mm)	u'/S_L	l/δ_L	Re	Ka	Da
A	1.0	0.8	2.395	0.387	2.16	1.03	112	9.74	0.478
B	1.0	∞	2.395	0.387	2.16	1.03	112	9.74	0.478
C	0.6	0.8	0.941	0.395	2.75	1.01	59	12.6	0.368