



Evaluation of a reduced mechanism for turbulent premixed combustion



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ABSTRACT

In this study, 3D direct numerical simulations of a multi-component fuel consisting of CO, H₂, H₂O, CO₂ and CH₄ reacting with air are performed. A freely propagating turbulent premixed stoichiometric flame is simulated for both low and high turbulence conditions i.e., the rms values of turbulent velocity fluctuations normalised by the laminar flame speed are of order 1 and 10. A skeletal mechanism involving 49 reactions and 15 species, and a 5-step reduced mechanism with 9 species, are used in order to evaluate the performance of the reduced mechanism under turbulent conditions. The 5-step mechanism incurs significantly lower computational expenses compared to the skeletal mechanism. The majority of species mean mass fractions and mean reaction rates computed using these two mechanisms are in good agreement with one another. The mean progress variable and heat release rate variations across the flame brush are also recovered by the reduced mechanism. No major differences are observed in flame response to curvature or strain effects induced by turbulence, although some differences are observed in instantaneous flame structure. These differences are studied using a correlation coefficient and detailed analysis suggests that this comes from the fluctuating heat release induced effects in the case with higher turbulence level. Further considerations based on instantaneous reaction rate and local displacement speed are discussed to evaluate the suitability of the reduced mechanism.

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1. Introduction

Natural hydrocarbon based fuel resources such as methane are finite, and are becoming increasingly more expensive to extract often requiring off-shore drilling at great depths. At the same time emission regulations are becoming stricter, due to increasing levels of CO₂ in the atmosphere. In light of these developments, low calorific value fuels such as Coke Oven Gas (COG), Blast Furnace Gas (BFG), and those coming from bio-gasifiers, are becoming increasingly popular as alternative fuels for power generation using industrial gas-turbines [1]. These are typically multi-component fuels, involving CO, H₂, H₂O, CH₄, CO₂, O₂ and N₂, with their compositions varying greatly depending on the production process [2–4].

The design of combustors operating efficiently, and in an environmentally-friendly manner to burn such fuels in turbulent flows is challenging. An integral part of the modern design process involves computational fluid dynamics (CFD) simulations of turbulent reactive flows. Three-dimensional direct simulations of turbulent reactive flows of practical interest, are still expensive despite the development of faster and efficient computers. This is primarily

due to two issues: (1) accurate description of the flow field requires to resolve the smallest dissipative scales, i.e., the Kolmogorov scale η_k , which requires an extremely prohibitive fine numerical grid, and (2) accurate description of the chemistry, requires the use of a very large detailed reaction set. A detailed reaction set usually involves more than hundreds of reactions and tens of species, even for a simple fuel such as CH₄, and the requirement for multi-component fuels is even larger. Furthermore, the time scales associated with each species can be very disparate, thus requiring the use of an extremely small time-step. All of the above factors, make such simulations impractical even on the fastest super-computer available to date.

Reynolds averaged Navier–Stokes (RANS) and Large Eddy Simulations (LES) approaches tackle the first issue on numerical and computational requirements. The second issue on the required chemical complexity, can be tackled in a variety of ways, using tabulated chemistry approaches [5–10], and chemistry reduction involving quasi steady state assumptions (QSSA), combined with partial equilibrium assumptions [11–19]. In schemes with QSSA, the computational effort is reduced considerably by introducing steady-state and partial equilibrium assumptions for particular species and reactions respectively. This reduces the number of species to be carried in simulations and the stiffness of the system by removing species with relatively short lifetimes.

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Usually, reduced mechanisms obtained using these approximations, are validated against laminar one-dimensional measurements such as the flame speed and ignition delay time. Following this validation procedure, such reduced mechanisms have been used in past Direct Numerical Simulation (DNS) studies [20–27], to gain insight for combustion sub-model development. This step entails a major assumption: that the reduced mechanism retains the same flame front structure and turbulence–flame interaction thereby yielding the same statistics as one would obtain using a detailed or a skeletal mechanism. This may or may not be correct and has not been validated yet in three dimensions, since most of the DNS studies in the past used either a single irreversible reaction or reduced chemical kinetics in three dimensional turbulence. Skeletal chemical kinetic mechanisms on the other hand were predominantly used in two dimensional simulations only, due to the high computational demand for three-dimensional simulations with detailed chemical complexity.

These investigations have been reviewed in many past studies [28–31], helping us to understand the role of chemical detail in turbulent combustion simulations. For example, it was shown in the 2D DNS of Baum et al. [32,33] that the responses of heat release rate and flamelet speed to curvature and tangential strain rate induced by turbulence on hydrogen–air premixed flames, were substantially different when a single or skeletal chemistry was used, although the general statistics such as the probability density function (pdf) of curvature did not vary much. The role of simulation dimensions was examined in detail in [34] where 2D simulations yielded much broader displacement speed pdfs in comparison with 3D simulations, with the discrepancies being proportional to the turbulence level u_{rms}/S_l , where S_l is the laminar flame speed. While the 3D simulations revealed the displacement speed to be strongly negatively correlated with curvature, the 2D data showed a much weaker correlation [34]. Since the displacement speed strongly depends on the flow field and mixture transport properties, it is expected that the type of chemical mechanism used will also affect this correlation and the respective pdfs through turbulence–chemistry interaction. This is particularly important from a modelling point of view since the displacement speed is involved in the G-equation and FSD modelling approaches. Furthermore, preferential diffusion effects of light species, are not described when a 1-step chemistry is used. The comparison of LES results with experimental data to assess the accuracy of reduced chemistry models [35], suffers from many additional assumptions introduced for the sub-grid scale combustion modelling. As a result, the exact influence of the chemical model employed, cannot be isolated unambiguously.

DNS studies are ideal to isolate the influence of chemical kinetics modelling on the flame structure and turbulence–chemistry interaction, and to test the performance of a particular chemical scheme for turbulent combustion. However, in the past, DNS studies of premixed combustion in simple canonical configurations with skeletal chemistry and archetypical configurations with reduced chemistry were predominantly used to gain insights on turbulence–chemistry interaction and model validation. A review of these studies in [28] suggests that three-dimensional DNS with adequate detail of chemical kinetics will be required to make general strides on the development of combustion sub-models for optimal design of future engines and fuels. The DNS of combusting flows in archetypical configurations with detailed chemistry and molecular transport for multi-component fuels is expected to be beyond the reach of even exa-scale computing. The use of skeletal or reduced mechanisms seems a plausible choice at this time.

Obviously, a reduced mechanism is preferred for computational reasons. However, the reduced mechanism must retain the essential features of flame structure, the relative role of various fuel species and important radicals, and their interactions with turbulence. The former aspects are usually verified using laminar flame measure-

ments and quantities computed using detailed or skeletal chemistry, as noted earlier. The turbulence–flame interaction aspects are usually presumed to hold. In this study, an attempt has been made to verify the ability of a reduced mechanism to capture the turbulence–flame interaction and flame front structure compared to a skeletal mechanism. This is achieved by performing 3D DNS of turbulent premixed combustion of a multi-component fuel mixture in a canonical configuration. The combustion chemistry is modelled using an extensively validated skeletal and 5-step reduced mechanism for multi-component fuel mixtures [36]. The details of these two mechanisms are given later in Section 2.1. The specific objectives of this study are (1) to compare the spatial distribution of heat release rate and species mass fractions in turbulent premixed flames computed using the skeletal and reduced mechanisms, (2) to study the respective statistics of mass fractions, reaction rates etc. obtained using these two mechanisms and (3) to examine the flame statistics, specifically pdfs of flame curvature, displacement speed, tangential strain rate, stretch rate and generalised flame surface density (FSD) which is closely related to the scalar dissipation rate of the reaction progress variable. These quantities are involved in combustion modelling based on flamelets approach.

The rest of the paper is organized as follows. The mathematical background and the numerical implementation are presented in Section 2 along with the computational parameters and the chemical schemes used. The results are presented and discussed in Section 3, and conclusions are drawn in the final section.

2. Mathematical background

2.1. Governing equations and numerical method

The direct numerical simulations have been conducted using the SENG2 code [37] which is a fully compressible code. The equations solved are those for the conservation of instantaneous mass, momentum, energy, and species mass fractions. These equations are written respectively as

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_k}{\partial x_k} = 0, \quad (1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_k u_i}{\partial x_k} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ki}}{\partial x_k}, \quad (2)$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial \rho u_k E}{\partial x_k} = -\frac{\partial p u_k}{\partial x_k} - \frac{\partial q_k}{\partial x_k} + \frac{\partial \tau_{km} u_m}{\partial x_k}, \quad (3)$$

and

$$\frac{\partial \rho Y_\alpha}{\partial t} + \frac{\partial \rho u_k Y_\alpha}{\partial x_k} = \dot{\omega}_\alpha - \frac{\partial \rho V_{\alpha,k} Y_\alpha}{\partial x_k}. \quad (4)$$

using common nomenclature. The symbol α denotes a species identifier. Further details of the above equations can be found in [37].

The thermal conductivity of the mixture, λ , is calculated using a relationship in [38], which is given as

$$\frac{\lambda}{C_p} = A_i \left(\frac{T}{T_0} \right)^r \quad (5)$$

where C_p is the specific heat capacity at constant pressure for the mixture. The model parameters are $A_i = 2.6246 \times 10^{-5} \text{ kg m}^{-1} \text{ s}^{-1}$ and $r = 0.6859$. The dynamic viscosity, μ , of the mixture is calculated by assuming a constant Prandtl number, Pr, through

$$\mu = \frac{\lambda}{C_p} \text{Pr} \quad (6)$$

From laminar unstrained flame calculations Pr = 0.7. The diffusion velocities for species are calculated using Fick's law:

$$\rho V_{\alpha,k} Y_\alpha = -\rho D_\alpha \frac{\partial Y_\alpha}{\partial x_k}. \quad (7)$$

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