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DNS of a turbulent lifted DME jet flame

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ABSTRACT

A three-dimensional direct numerical simulation (DNS) of a turbulent lifted dimethyl ether (DME) slot jet flame was performed at elevated pressure to study interactions between chemical reactions with low-temperature heat release (LTHR), negative temperature coefficient (NTC) reactions and shear generated turbulence in a jet in a heated coflow. By conditioning on mixture fraction, local reaction zones and local heat release rate, the turbulent flame is revealed to exhibit a “pentabrachial” structure that was observed for a laminar DME lifted flame [Krisman et al., (2015)]. The propagation characteristics of the stabilization and triple points are also investigated. Potential stabilization points, spatial locations characterized by preferred temperature and mixture fraction conditions, exhibit autoignition characteristics with large reaction rate and negligible molecular diffusion. The actual stabilization point which coincides with the most upstream samples from the pool of potential stabilization points fovr each spanwise location shows passive flame structure with large diffusion. The propagation speed along the stoichiometric surface near the triple point is compared with the asymptotic value obtained from theory [Ruetsch et al., (1995)]. At stoichiometric conditions, the asymptotic and averaged DNS values of flame displacement speed deviate by a factor of 1.7. However, accounting for the effect of low-temperature species on the local flame speed increase, these two values become comparable. This suggests that the two-stage ignition influences the triple point propagation speed through enhancement of the laminar flame speed in a configuration where abundant low-temperature products from the first stage, low-temperature ignition are transported to the lifted flame by the high-velocity jet.

1. Introduction

Partially premixed combustion is prevalent in many combustion applications, for example, in the lift-off stabilization of a diesel jet flame. It nominally consists of fuel rich and fuel lean premixed flames and a trailing diffusion flame which consumes excess fuel and oxidizer originating from the premixed branches. This so-called triple flame structure is observed when the reactant temperature is sufficiently low so as to preclude the possibility of autoignition, in both stationary and non-stationary configurations [3]. While the structure is often masked in a turbulent flow due to significant strain and high mixing rates, its presence is revealed in mixture fraction and progress variable coordinates. The diesel engine is one such application where fuel and air are partially premixed. In diesel engine combustion, fuel is injected into a hot cylinder at a high velocity, and once the mixture is ignited a lifted flame is established. As many studies have reported [4–6], the flame structure and stabilization of a lifted flame depends on a balance between mixing and chemical reaction modulated by large scale flow structure, which is difficult to generalize. For example, two previous direct numerical simulations of turbulent lifted hydrogen jet flames show very different flame structures [7,8]. In addition to the competition between mixing, chemical reaction and global flow structure, there are additional complexities that can influence overall flame behavior in diesel combustion. The complexities arise due to the chemical kinetic characteristics observed in large hydrocarbon fuels, that is, the two-stage ignition and negative temperature coefficient (NTC). At sufficiently low injector temperatures diesel fuels undergo a two-stage ignition process comprised of low- and high-temperature ignition. The majority of the heat release is a result of the high-temperature ignition, similar to single-stage ignition fuels, whereas the low-temperature ignition is slightly exothermic, generating a small amount of low-temperature heat release (LTHR). The significance of low-temperature ignition, however, is that it also generates low-temperature species that could potentially influence the overall reactivity of the fuel mixture. Negative temperature coefficient regime is observed over a

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range of mixture temperatures, determined by the thermochemical condition. The ignition delay time increases with increasing temperature inside the NTC regime, whereas it decreases with increasing mixture temperature outside of this temperature range. The non-monotonic behavior of ignition delay time could directly affect the lift-off length, particularly if the lifted stabilization mechanism is governed by autoignition [8]. NTC behavior has the potential to further alter emissions and efficiency performance in a diesel engine through its affect on the lift-off length [9,10].

Recently, a parametric study of two-dimensional Direct Numerical Simulations (DNS) of shear-less laminar lifted dimethyl ether (DME) flames at a nominal engine pressure and temperatures has revealed the existence of a "*pentabrachial*" flame structure when a lifted flame is established under strong LTHR and NTC conditions with a relatively high oxidizer temperature [1]. A similar result is also reported in Ref. [11]. As explained in detail later in Section 3.1, the pentabrachial flame consists of two upstream flame branches due to LTHR and NTC in addition to a conventional triple flame further downstream. Also, the stabilization point of the lifted flame shifts towards fuel-lean conditions due to NTC. The existence of five flame branches may influence the overall flame behavior including the triple flame propagation speed. In turbulent flows, observation of such distinct flame branches established in partially premixed combustion is generally difficult due to strong turbulence–flame and flame–flame interactions [4,8,12], although a turbulent lifted hydrogen jet flame reported in Ref. [7] exhibits a clear triple flame structure in physical space.

In the present study, the focus is on the interactions between chemical reactions with LTHR and NTC, and sheared turbulence in a planar jet. Specifically, does a pentabrachial structure still exist under the presence of flame–flame and turbulent–flame interactions caused by strong turbulence? Moreover, what is the effect of two-stage ignition and NTC chemistry on the overall flame stabilization? Insights into these questions extend the previous understanding of laminar DME lifted flames [1]. For this purpose, a three-dimensional DNS of a turbulent lifted DME slot jet flame has been performed at elevated pressure. Although the present pressure is still far from nominal engine conditions due to computational limitations, the fuel and oxidizer temperatures are carefully chosen to include LTHR and NTC effects.

The present paper is organized as follows: the numerical methods used to perform the present simulations are described in Section 2, followed by a detailed description of the DNS configuration and numerical and thermochemical conditions. The flame structure, the flame propagation characteristics and the effect of two-stage ignition are discussed in Section 3. The conclusions are made in Section 4.

2. Direct numerical simulations

The Sandia DNS code S3D [13] is used to simulate DME/air combustion. The code solves the fully-compressible conservation equations for mass, momentum, total energy and species continuity. The chemical reactions are described by a reduced mechanism for DME-air combustion involving 30 species developed in a previous study [14]. The present reduced mechanism is derived from a detailed chemical kinetic reaction mechanism [15], and includes key kinetic mechanisms for DME combustion. DME is primarily consumed by hydrogen abstraction by OH

$$CH_3OCH_3 + OH = CH_3OCH_2 + H_2O, \tag{R1}$$

but also by HO_2 under elevated pressure and intermediate temperature conditions

$$CH_3OCH_3 + HO_2 = CH_3OCH_2 + H_2O_2, \tag{R2}$$

as reported previously [16,17]. The CH_3OCH_2 radicals undergo oxygen addition at low temperature as

$$CH_3OCH_2 + O_2 = CH_3OCH_2O_2. \tag{R3}$$

The equilibrium of this reaction is strongly temperature dependent, which favors methoxymethyl-hydroperoxy ($CH_3OCH_2O_2$) at low temperatures. Thus, $CH_3OCH_2O_2$ is a good marker for low-temperature chemical kinetics. Once the low-temperature process is suppressed by accumulated heat release due to LTHR, thermal decomposition of CH_3OCH_2 begins, which produces radicals that consume the remaining fuel and intermediates species, producing intense chemical reactions and heat. Nitrogen is inert in this context and therefore, NO_x formation reactions are not included. The species specific heats are modeled as polynomial functions of temperature as described in CHEMKIN and TRANSPORT, and mixture-averaged transport coefficients are used [18,19]. Radiative heat transfer is not considered in the present simulations. Spatial derivatives are obtained using an eighth-order central finite difference scheme which gradually reduces to a third-order one-sided difference stencil on the open domain boundaries [20]. A tenth-order explicit spatial filter is applied to remove any spurious high-frequency fluctuation in the solution [20]. Time integration is achieved using a six-stage fourth-order explicit Runge–Kutta method [20].

2.1. Thermochemical condition

Diesel (surrogate) fuels are by nature highly reactive. In nominal diesel engine combustion conditions, the reactant mixture is even more reactive due to increased pressure and temperature. In an engine-relevant configuration, a high speed jet (typically ∼400 m/s issuing from the injector) yields a large lift-off length typically ∼100 times the nozzle diameter, even in such a highly reactive environment. In partially premixed combustion, especially at engine conditions, a reactant mixture is exposed to several turbulence/combustion phenomena as it proceeds towards its lift-off position. They include mixing of reactants with high-temperature oxidizer due to strong velocity and scalar gradients and LTHR that creates radical pools for subsequent high-temperature reactions. Some of these conditions require immense computational resources that are not currently feasible for DNS. For example, a highly reactive fuel at high pressure yields very thin reaction layers that require extraordinarily fine spatial resolution (small mesh size Δx). Similarly, a large jet velocity close to sonic *Ma* that generates large velocity gradients also imposes fine turbulence scales. One way to alleviate the enormous spatial resolution requirements is through fuel dilution, which also permits a sufficient lift-off length for mixing and LTHR to occur and to achieve strong turbulence-flame interactions within a feasible DNS domain length considerably shorter than 100 nozzle diameters.

The mixture in the present fuel and oxidizer stream, respectively consists of $0.1DME+0.9N_2$ and $0.21O_2+0.79N_2$. Comparing previous DME jet flames in Ref. [1] the present fuel stream is heavily diluted. This results in a larger stoichiometric mixture fraction, $\xi_{st} = 0.42$, shifted well into the fuel jet stream. Under the present moderately elevated pressure of 5 atm, the high level of dilution results in a spatial resolution governed by comparable minimum reaction layer thickness and the Kolmogorov scale (discussed in Section 2.4), and hence, maximizing turbulence-flame interaction while maintaining a feasible computational cost. Also, the temperature for each stream is carefully chosen to achieve both LTHR and NTC; they are chosen to be 500 K and 1000 K for the fuel and oxidizer streams, respectively. With these mixture compositions and temperatures for the present fuel and oxidizer streams, zero-dimensional homogeneous ignition simulations are performed