3D DNS of MILD combustion: A detailed analysis of heat loss effects, preferential diffusion, and flame formation mechanisms

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ABSTRACT

Moderate or intense low oxygen dilution (MILD) combustion is a relatively new technology which combines low emissions with high efficiency. As the name suggests, it requires high degrees of dilution in addition to preheating of the reactants using the combustion products. It has been applied to industrial burners for some time, but the complex physical mechanisms are yet to be resolved to extend the application to other areas. In this study, our aim is to analyze MILD combustion conditions to reveal the mentioned physical phenomena and their interactions. To this end, direct numerical simulations (DNS) in the form of autoigniting mixing layers are conducted, and the results are thoroughly analyzed. Conditions used in the simulations are taken from the jet in hot coflow experiments, which are designed to mimic MILD conditions. Detailed chemistry and transport models are employed in the numerical tools to fully understand the interactions of turbulence, molecular diffusion and chemical reactions. In addition, temperature variations due to heat loss effects in the experiments are taken into account. We have found that the heat loss and preferential diffusion effects are crucial in predicting not only the ignition delay, but also the flame structures and heat release rates. In addition, it is found that the flame formation is initiated by autoignition with different ignition delays along the most reactive mixture fraction, instead of a flame propagation following an initial autoignition spot. The findings of this study will broaden the knowledge on MILD combustion, and provide useful insight in developing reduced turbulence and chemistry models in the future.

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1. Introduction

In combustion devices, it is desirable to increase efficiency and decrease harmful emissions. Moderate or intense low-oxygen dilution (MILD) combustion is a promising concept to achieve these goals. The combustion process is considered as MILD when the preheating is so high that the temperature of the reactants is higher than the autoignition temperature, and the dilution is high enough that the increase of the temperature in the combustor is less than the autoignition temperature (in Kelvin) [1]. The efficiency increases because the excess heat in the products is used, and the emissions decrease because the maximum temperature in the combustion chamber is decreased as a result of the high dilution. In addition, combustion takes place uniformly and silently, and there occurs no visible flame in the MILD combustion regime

[1–3]. It is also referred to as flameless oxidation (FLOX) [4], or high temperature air combustion (HiTAC) [5] in the literature.

MILD combustion has received increasing attention in the recent years due to its beneficial characteristics like high efficiency and low emission of the pollutants CO [6] and NO_x [7]. There have been several experimental investigations to mimic and analyze the MILD conditions. One of the most used experimental setups to study MILD combustion is the jet in hot coflow (JHC) configuration. JHC was studied under both laminar [8,9] and turbulent [10,11] conditions. In this type of burner, a fuel jet is issued into a hot and diluted coflow, and the lifted flame is stabilized by autoignition. In [11], Oldenhof et al. used natural gas as fuel and the products of a rich-operated secondary burner as oxidizer, which has an oxygen content of 7–10% by mass. They varied the jet Reynolds number and observed that the lift-off height decreased with increasing jet Reynolds number due to enhanced entrainment. Dally et al. [10] used methane–hydrogen mixture with equal amounts by volume as fuel, and changed the oxygen content from 3% to 9% by mass. They found that the peak temperature rises and the lift-off height decreases with increasing oxygen content.

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JHC burners have also been studied extensively by the numerical community. Different Reynolds Averaged Navier–Stokes (RANS) [12,13] and large eddy simulation (LES) [14–16] studies were performed under turbulent conditions. De et al. [12] used eddy dissipation concept (EDC) to simulate the experiments of Oldenhof et al. [11]. They predicted the radial profiles of temperature and velocity reasonably well, but failed to match the lift-off heights found in the experiments. Christo and Dally [13] modeled the flame in [10] employing different turbulence and chemistry models. They concluded that the EDC with the standard $k - \epsilon$ turbulence model produces the best agreement with the experimental results, and differential diffusion effects should be taken into account. In [14], Kulkarni and Polifke applied a flamelet/progress variable (FPV) approach and found that the heat losses in the coflow are crucial in determining lift-off height. Afarin and Tabejamaat [15] investigated the effect of the initial turbulence level in the fuel. They used three different turbulence intensities of 4%, 7% and 10%, and obtained the best agreement with the experimental results using 4% initial turbulence intensity. Ihme et al. [16] employed an FPV formulation with a three stream approach to account for the outermost cold air stream in the experiments of Dally et al. [10]. They also adjusted the controlling variables to accurately represent the species profile of the coflow. In their computations, addition of the third stream yielded satisfactory results in terms of temperature and species profiles.

Although the aforementioned numerical studies have provided valuable information regarding MILD combustion, they rely on models for turbulence and chemistry, and do not resolve the smallest scales of flow and flame structures. To reveal the complex physical interaction between turbulence, chemistry, and diffusion; it is required to fully resolve the mentioned physical phenomena, i.e., a direct numerical simulation (DNS) study must be conducted. Thorough 3D DNS calculations of autoignition of a fuel jet in a heated coflow were performed by Yoo et al. [17,18]. In [17], they observed that the main source of flame stabilization is autoignition, and downstream of the flame base, premixed and non-premixed flames coexist with autoignition. However, their conditions do not represent MILD combustion since the oxidizer was not diluted. Van Oijen [19] performed 2D DNS of autoigniting mixing layers representative of JHC burner in [10] and compared the results with 1D diffusive layer simulation results. His results show that the ignition delay times for the diffusive layer simulations and the 2D DNS are almost the same, and they are strongly dependent on the preferential diffusion effects. Nevertheless, real turbulence effects could not be reproduced in his study since the 2D turbulence lacks vortex stretching phenomenon and has an inverse energy cascade. In addition, heat loss and the resulting non-uniform temperature profile of the coflow were not taken into account. These two factors can have strong effects on the physics of the problem. To our knowledge, the only 3D DNSs of MILD combustion were carried out by Minamoto et al. [20,21]. They simulated a premixed MILD system whose composition is obtained via 1D laminar flames, and compared the results with a conventional premixed case to examine differences in flame structures. They concluded that there are strong chemically reacting zones in the MILD regime, but unlike traditional premixed flames, the reaction layers are not sheet like and they interact with each other. Although their studies shed light on MILD combustion flame structures for premixed cases, they do not provide any interpretation for spontaneous mixing and chemistry, which is the case in many MILD systems including JHC experiments.

In the present study, the physical phenomena and their interactions in the MILD combustion were explored by performing DNS computations with detailed chemistry and constant Lewis number approach. The influence of non-uniformities in the temperature and species profiles were investigated, and the effects of preferential diffusion were carefully examined. Flame formation mechanisms and characteristics at the ignition kernels in a MILD combustion system of non-premixed type were revealed.

In the following parts of the paper; the numerical approach is explained, detailed information on simulated cases is given, the results are presented and discussed, and finally some conclusions are drawn.

2. Numerical method and simulation setup

In the DNS code [22–24], the governing equations are solved in fully compressible forms in terms of density ρ, velocity u_j, pressure p, species mass fractions Y_α, and temperature T:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0, \tag{1}$$

$$\rho \frac{\partial u_j}{\partial t} + \rho u_i \frac{\partial u_j}{\partial x_i} = -\frac{\partial p}{\partial x_j} + \frac{\partial \sigma_{ij}}{\partial x_i}, \tag{2}$$

$$\rho \frac{\partial Y_\alpha}{\partial t} + \rho u_i \frac{\partial Y_\alpha}{\partial x_i} = -\frac{\partial}{\partial x_j}\left(\frac{\lambda}{Le_\alpha c_p}\frac{\partial Y_\alpha}{\partial x_j}\right) + \omega_\alpha, \qquad (\alpha = 1, \ldots, N-1) \tag{3}$$

$$
\begin{aligned}
\rho c_v \frac{\partial T}{\partial t} + \rho c_v u_i \frac{\partial T}{\partial x_i} = &-\frac{\partial}{\partial x_j}\left(\lambda \frac{\partial T}{\partial x_i}\right) - p\frac{\partial u_i}{\partial x_i} + \sigma_{ij}\frac{\partial u_i}{\partial x_j} \\
&+ \frac{\partial}{\partial x_i}\left(\sum_{\alpha=1}^{N-1} h'_\alpha \frac{\lambda}{Le_\alpha c_p}\frac{\partial Y_\alpha}{\partial x_i}\right) \\
&- \sum_{\alpha=1}^{N-1}(h'_\alpha - R'_\alpha T)\left[\omega_\alpha + \frac{\partial}{\partial x_i}\left(\frac{\lambda}{Le_\alpha c_p}\frac{\partial Y_\alpha}{\partial x_i}\right)\right], \tag{4}
\end{aligned}
$$

where c_v is specific heat at constant volume and λ is thermal conductivity of the mixture, σ is stress tensor, Le_α and ω_α are the Lewis number and source term of species α. Eq. (3) is solved for $N - 1$ species excluding N_2, and diffusion correction is imposed by $\sum Y_\alpha = 1$. To account for the diffusion correction in Eq. (4), enthalpy and gas constant for each species are defined as $h'_\alpha = h_\alpha - h_{N_2}$ and $R'_\alpha = R_\alpha - R_{N_2}$, and the summation terms are computed for $N - 1$ species.

As can be seen from Eq. (4), viscous dissipation is taken into account. However, heat flux due to the mass diffusion (Dufour effect), species diffusion due to temperature gradient (Soret effect), and the diffusion of species due to pressure gradients are neglected. In order to close the Eqs. (1)–(4) a state relationship is required. In this study, the ideal gas law is used:

$$p = \rho R T \sum_{\alpha=1}^{N} Y_\alpha / M_\alpha, \tag{5}$$

where R is the universal gas constant and M_α is the molar mass of species α.

For the calculation of the source terms ω_α, enthalpies h_α and heat capacities c_p and c_v, the DRM19 reaction mechanism [25], which includes 21 species (H_2, H, O, O_2, OH, H_2O, HO_2, CH_2, $CH_2(S)$, CH_3, CH_4, CO, CO_2, HCO, CH_2O, CH_3O, C_2H_4, C_2H_5, C_2H_6, N_2, AR) and 84 reactions, was used. The DRM19 mechanism is a reduced version of the GRI 1.2 mechanism [26], and was tested and validated against the GRI mechanisms in terms of ignition delay and laminar flame speed. It provides a good compromise between accuracy and computational cost. Thermal conductivity λ and viscosity μ coefficients of the mixture are computed with simplified relations using the heat capacity and temperature of the mixture: