Large-Scale Quasi-DNS of Mixed-Mode Turbulent Combustion

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In many applications like gas turbines, the combustion process can take place in partially-premixed environments, where fuel and oxidizer are not fully mixed before combustion. These partially-premixed or mixed-mode flames have become a focus of combustion research in the last few years. In this work, a quasi-DNS of an experimentally measured burner configuration has been conducted. The simulation employs a complex reaction mechanism and detailed molecular diffusion coefficients for each chemical species. Due to the highly resolved numerical grids and the detailed thermo-physical and chemical properties, the simulation results allow to characterize the flame with the help of flame markers in greater detail than the experiments can provide. The investigated flame exhibits characteristics of a premixed flame near the nozzle. Further downstream both premixed and non-premixed combustion modes become equally important in terms of the heat release rate. The dataset from the simulation also allows to form joint probability density functions of commonly used control variables to study their correlations depending on the combustion regime.

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1 Introduction

In technical combustion devices, fuel and oxidizer are often not perfectly mixed. Therefore, the combustion exhibits both regions with premixed and non-premixed modes. Because of this, many combustion models, which are derived for only one combustion mode, fail to predict properties of these mixed-mode flames correctly. In this work, a quasi-DNS of the experimentally investigated “Sydney” burner in configuration FJ200-5GP-Lr75-57 [1,2] was performed. This burner configuration was created specifically to investigate mixed-mode flames. It consists of a retractable inner fuel pipe, an annular oxidizer pipe and a surrounding hot pilot flow. The more the inner fuel pipe is retracted, the more the flame becomes a premixed flame; the more it is pushed forward, the less time air and fuel have to mix and it becomes a diffusion flame.

2 Numerical Setup

The simulation of the Sydney burner is a quasi-DNS, which means that the reactive flow is computed without any sub-grid models for the turbulence or combustion. Instead, all length and time scales of the reactive flow are resolved in the region where experimental data are available. The simulation is conducted in three steps: 1) A precursor highly-resolved LES for the flow in the fuel and oxidizer pipes to initialize 2) a non-reactive quasi-DNS for the partial mixing of methane and air and 3) a reactive quasi-DNS of the hot pilot igniting the partially premixed methane/air flame downstream. The inner diameter of the fuel-air nozzle is \( D = 7.5 \text{ mm} \). Both quasi-DNS from step 2) and 3) are performed on numerical grids with 150 million cells each, with a smallest grid size of 5 \( \mu \text{m} \). The quasi-DNS include detailed molecular diffusion coefficients for each chemical species based on rigorous kinetic gas theory and the Hirschfelder-Curtiss approximation [3].

For the chemical reaction rates, finite rate chemistry from a complex reaction mechanism by Lu et al. [4] was applied consisting of 19 chemical species and 11 additional species that are assumed to be in a quasi-steady state. The temporal discretization is implicit and second order in time. For the spatial discretization, a fourth order interpolation scheme with low numerical dissipation is used. The simulation has been run on the German national supercomputer “Hazel Hen” [5] on up to 28,800 CPU cores with a custom chemistry implementation which increases the performances of reaction rate computations [6].

The simulations are performed with the open-source library OpenFOAM [7] in version v1712, which provides general tools for computational fluid dynamics applications. It is used to solve the fully compressible Navier-Stokes equations as well as the conservation of energy and mass for all chemical species. Thermo-physical properties of the gas mixture are computed with the open-source library Cantera [8].

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3 Results

Fig. 1: Left: Time averaged heat release rate $\dot{Q}$ integrated over volume segments with $\Delta x = 1$ mm from premixed and non-premixed combustion regimes along the axial direction. Right: JPDF of reaction progress $c$ and mixture fraction $Z$ at a single location (middle) and the same JPDF from non-premixed contributions only (right).

4 Flame Marker and Characterization of the Flame

In the past, different markers for identification of the combustion regimes have been developed. In this work, premixed and non-premixed regimes are identified by the flame index $FI$ [9]

$$FI \equiv \frac{\nabla Y_{CH_4} \cdot \nabla Y_{O_2}}{|\nabla Y_{CH_4} \cdot \nabla Y_{O_2}|}$$  \hspace{1cm} (1)

where $Y_{CH_4}$ and $Y_{O_2}$ are the mass fractions of methane and oxygen. The flame index only takes values of unity, when fuel and oxidizer gradients are aligned and the flame shows characteristics of premixed flames, and negative one if the flame corresponds to a non-premixed flame. This allows to characterize the flame. In Fig. 1 on the left, the heat that is released by regions with $FI = 1$ and $FI = -1$ is depicted. The results show that the flame is dominated by premixed combustion characteristics near the nozzle ($x/D < 10$) and further downstream both combustion regimes become equally important.

The simulation results also allow to study the correlation of commonly used control variables like mixture fraction $Z$ and reaction progress $c$. In the middle of Fig. 1, the joint probability function (JPDF) of these two control variables is depicted. It was obtained from time series at a single location within the flame at $x/D = 15$. The JPDF shows a strong correlation between $Z$ and $c$. On the right of Fig. 1, the same JPDF as in the middle is shown, where only pairs of $Z$ and $c$ are included when $FI = -1$. This demonstrates that the non-premixed combustion is present mostly in regions with high $Z$ at this position.

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