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Full Length Article

Large Eddy Simulation of CO_2 diluted oxy-fuel spray flames

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ABSTRACT

We report results of a computational study of oxy-fuel spray jet flames. An experimental database on flames of ethanol burning in a coflow of a O_2–CO_2 mixture, created at CORIA (Rouen, France), is used for model validation (Cléon et al., 2015). Depending on the coflow composition and velocity the flames in these experiments start at nozzle (type A), just above the tip of the liquid sheet (type B) or are lifted (type C) and the challenge is to predict their structure and the transitions between them. The two-phase flow field is solved with an Eulerian–Lagrangian approach, with gas phase turbulence solved by Large Eddy Simulation (LES). The turbulence-chemistry interaction is accounted for using the Flamelet Generated Manifolds (FGM) method. The primary breakup process of the liquid fuel is neglected in the current study; instead droplets are directly injected at the location of the atomizer exit at the boundary of the simulation domain. It is found that for the type C flame, which is stabilized far downstream the dense region, some major features are successfully captured, e.g. the gas phase velocity field and flame structure. The flame lift-off height of type B flame is over-predicted. The type A flame, where the flame stabilizes inside the liquid sheet, cannot be described well by the current simulation model. A detailed analysis of the droplet properties along Lagrangian tracks has been carried out in order to explain the predicted flame structure and discuss the agreement with experiment. This analysis shows that differences in predicted flame structure are well-explained by the combined effects of droplet heating, dispersion and evaporation as function of droplet size. It is concluded that a possible reason for the difficulty to predict the type A and B flames is that strong atomization-combustion interaction exists in these flames, modifying the droplet formation process. This suggests that atomization-combustion interaction should be taken into account in future study of these flame types.

1. Introduction

Since in many combustion processes the main source for NOx formation is the oxidation at high temperature of the N_2 contained in air, a natural suggestion to reduce or eliminate the NOx emission, has been to separate N_2 and O_2 and use enriched air or pure O_2 as oxidiser. This is the concept of oxy-fuel combustion. This combustion technology has many advantages. In case of 100% pure oxygen and in absence of fuel bound nitrogen, NOx emission is no longer an issue. Second, the flue gas of this combustion process is predominantly CO_2 and H_2O, by separating water vapor through cooling or compression, a CO_2 stream for carbon capture and sequestration (CCS) is available. Such a zero emission combustion system, is particularly appealing.

However, oxy-fuel combustion also faces several challenges. First of all, N_2 separation from air with current technologies is energy consuming and expensive. Second, switching to oxy-fuel combustion drastically changes the process conditions. Adiabatic flame temperature of combustion with O_2 is high and the resulting high local heat flux implies a heavy thermal load to the burner. Third, due to the high temperature, a small amount of N_2 remaining after incomplete separation has a large chance to be converted to NOx. Less severe conditions with moderate heat flux and lower emissions can be created by dilution of the O_2 with part of the produced CO_2. The level of dilution appears as a process variable and research is still needed to find optimal the oxy-fuel combustion technology to be used in practical systems.

Local structure in spray flames can have a variety of types depending on the relative time scales of the process involved. This has been systematically reviewed recently by Sanchez et al. [2]. Detailed numerical simulations reveil the mechanisms leading to the different structures. Reveillon and Vervisch [3] did pioneering

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work by reveal the dilute spray flame structure using 2D DNS. They reviewed earlier spray flame regime diagrams and presented a new classification based on three dimensionless quantities: the fuel/air equivalence ratio within the core of the spray jet, the mean inter-droplet distance to flame thickness ratio, and the evaporation time to flame time ratio. In jet-in-coflow flames these parameters can be influenced by changing fuel injection and coflow conditions. The influence of varying oxygen concentration in the coflow has been the subject of a limited number of studies in the literature. A number of references have addressed the range of oxygen concentrations lower than air. Reddy et al. [4] studied the variation in flame structure experimentally using kerosine as fuel and comparing flame structure as function of fuel injection pressure and coflow composition. Their study includes cases with oxygen percentage in the coflow varying from 21% down to 17%. The database of the Delft spray in coflow flames [5] covers cases with air as coflow and cases with hot diluted coflow with oxygen percentage around 10%. An extensive study on ethanol spray combustion in a coflow consisting of only O_2 and CO_2, and covering a very wide range of oxygen concentration from 25% to 80% was done at CORIA (CNRS, University of Rouen and INSA of Rouen) and reported by Cléon et al. [1]. The goal of the present work is to report results of a computational study of the CORIA experiments. In the next sections we respectively describe the experimental setup and the simulation method Section 2, analysis of the results Section 3 and conclusions Section 4.

2. Modeling approach

2.1. Experimental setup & Simulation detail

In this study we simulate jet-in-coflow flames from the CORIA oxy-fuel spray combustion database [1]. Fig. 1 shows the dimension of the furnace in which the experiment was carried out and also shows the cross section of the computational domain, discussed below. The database concerns a series of flames with different combinations of coflow velocity and CO_2 dilution level of the oxidiser. A parameter α is used to characterize the degree of dilution of O_2 by CO_2, and is defined as follows:

$$\alpha = \frac{X_{CO_2}}{X_{CO_2}} + X_{O_2} \times 100\%, \quad (1)$$

where X denotes the mole fraction. In the experiment, the coflow velocity was changed by varying the coflow exit area with different insert units. In this way the coflow mass flow rate could be kept constant while varying the velocity [1]. Here we consider cases with two different coflow inserts, namely "insert 95" and "insert 200", respectively having coflow annulus outer diameter 95 mm and 200 mm and corresponding coflow mean velocity 0.51 m/s amd 0.11 m/s, respectively. For each insert we consider a case with $\alpha = 40$ and a case with $\alpha = 60$. An overview of the characteristics of the four case is given in Table 1.

In the experiments three types of flame structure have been observed, differing in the relative distance of the flame base to the atomization region [1]. The "type A" and "type B" flames are observed in cases with relatively small α (e.g. 40). The "type A" flame is anchored at the nozzle by a small conical central flame, while the main flame stabilizes at the tip of the liquid sheet. The type B flame, found at higher coflow velocity, consists only of the main flame and anchors at the tip of the liquid sheet. Finally for larger α, e.g. $\alpha = 60$, also "Type C" flame is observed, which stabilizes at far downstream of the dense region.

One of the flames in the database (case $\alpha 60 - I95$) has been simulated by Enjalbert [6] using massively parallel computing emplying the YALES2 solver and using LES with tabulated chemistry. In that simulation the computational domain covered the entire furnace interior, and the computation was done using a mesh with 27 M cells on 1024 processors and using a finer mesh with 215 M cells on 8192 processors. That study reached qualitative agreement of flame structure, but it also made clear that the modeling of the spray inlet conditions for this experiment is an important issue.

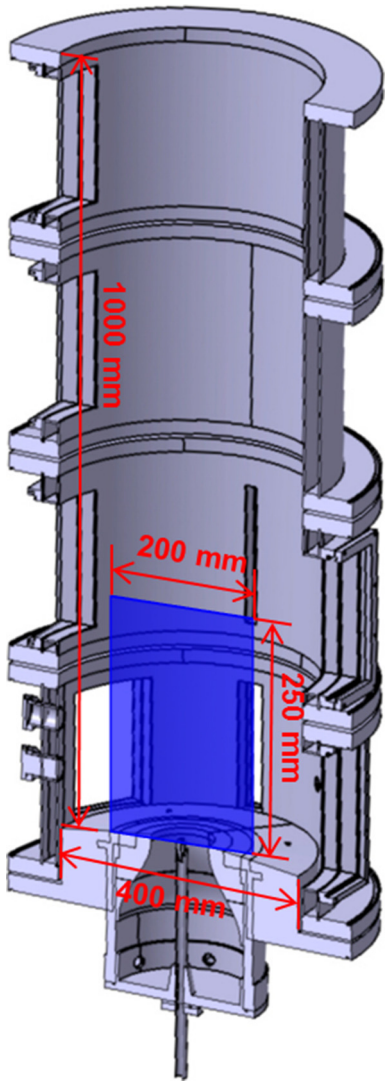

Fig. 1. Experimental set up with the illustration of the dimensions [1]. The blue region shows a cross-section of the computational "small" domain.

The simulation in this study is carried out using the open source CFD package — OpenFOAM [7]. New libraries have been created for the FGM storage and retrieval algorithms and are dynamically linked to a customized solver for spray combustion. The new solver is referred to as "sprayFGMFoam". This new solver has been successfully applied earlier in the modeling of MILD spray flames from the DSHC dataset, created at Delft University of Technology [8,9]. We use LES with tabulated chemistry (FGM) and the simulations have been performed on 100 processors of Cartesius, the Dutch supercomputer. As a first step study, in this paper we are only interested in the near field structure of the spray flames, therefore a smaller computational domain is adopted, illustrated in Fig. 1. In order to study the influence of the computational domain and mesh resolution, three different meshes have been adopted; details are listed in Table 2.