Assessment of combustion paradigms for modeling a cyclonic burner under MILD Combustion conditions

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Abstract
The development of MILD Combustion systems in several practical applications is hampered by a lack of understanding into such regime and thus novel tools are required compared to conventional combustion systems. In MILD combustion technologies, reactants are diluted with large amounts of burnt reaction products prior to ignition, which enables reactive structure stabilization under diluted conditions, thereby avoiding high-temperature regions that promote enhanced thermal NOx formation. In this background, computational fluid dynamics (CFD) for the prediction of the burner behavior and its optimization, appears essential for a successful introduction of such a concept in some industries. A major issue in the modeling of diluted combustion is the pronounced sensitivity of the reactive structure to the reaction chemistry and therefore detailed kinetic schemes are necessary when a gas mixture is subjected to dilution by hot reaction products.
In order to include detailed chemistry in fluid-dynamics simulations several turbulent combustion models were used and they are represented by the Eddy Dissipation Concept (EDC), PaSR and the Flamelet Generated Manifold (FGM). In particular, this study investigates the combustion characteristics of MILD Combustion in a novel cyclonic lab-scale burner. The numerical computations were performed incorporating turbulent combustion models in RANS simulations in order to determine the effect of several different main parameters such as inlet oxidizer temperature, and mixture composition on models performance.
Therefore, an assessment of models was carried out on the basis of an experimental/numerical comparison by evaluating the temperature inside the burner for a fixed condition. Results suggest that both the modified EDC and PaSR represent promising tool for modeling the complex flame structures of cyclonic MILD burner, although in several conditions they depict some aspects that need to be further investigated.

Introduction
Enhancement of thermal efficiency with fuel flexibility and ultra-low emissions is one of the most challenging area for combustion researchers. Among the new

technologies, MILD combustion [1] seems to be one of the most promising. Such operating conditions feature a process with a distributed reaction zone, relatively uniform temperatures within the combustion chamber, no visible flame, low noise, negligible soot formation and very low NO_x and CO emissions [2]. In recent years, attention has been paid to MILD combustion modeling, due to the very strong coupling between turbulence and chemistry of such a combustion regime. The flue gas entrainment increases the inert content of the fresh mixture so that chemical kinetics become slow enough with time scales comparable to the mixing ones [3]. Therefore, the turbulence/chemistry interaction need to be considered with appropriate and effective turbulent combustion models [4]. The poor knowledge of MILD reaction zones also calls into question the common use of both flamelet-like and non-flamelet-based turbulent combustion models for Reynolds-Averaged Navier-Stokes (RANS) simulations [5] and for Large Eddy Simulations (LES) [6]. The use of CFD tools to understand burner behaviour and to design its optimization appears essential, both for describing turbulent mixing and chemical reactions. Attractive strategies for including detailed chemistry effects using moderate CPU resources are tabulated chemistry techniques. Among such models, there are flamelet generated manifold (FGM) [7] techniques, based on Flamelet approach. In particular, Abtahizadeh et al. [8] showed that Igniting Mixing Layers (IML) type flame is the best option for representing MILD combustion in a jet in hot coflow (JHC) burner.
On the other hand, more complex turbulence/chemistry interaction models have been proposed in literature and successfully applied to MILD. Among them, it is worth to mention the Eddy Dissipation Concept (EDC) [9], which splits every computational cell into two regions: the fine structures, modeled as Perfectly Stirred Reactors (PSR), and the surrounding fluid mixture. Recently, Aminian et al. [10]. have shown the importance of adjusting the fine structure residence time constant (C_τ) simulating MILD combustion. Partially-Stirred Reactor (PaSR) model, originally proposed by Chomiak [11], is an extension of EDC and is characterized by a different definition of the reacting volume fraction, which becomes the ratio between the chemical time scale and the sum of mixing and chemical scales. It has been successfully applied to MILD combustion in the Adelaide Jet in Hot Co-flow (JHC) by Ferrarotti et al. [12]. Although significant progress has been achieved for MILD combustion modeling, there are still important issues concerning the reactive structures, the turbulence-chemistry interaction and the effect of fuel composition, which need to be addressed. The elucidation of the above topics needs high fidelity and comprehensive experimental data to validate the numerical models. In the past, Jet in Hot Coflow (JHC) configuration [13], and the Cabra flame [14] have been conceived to emulate flameless conditions by feeding diluted and hot streams to the burner. The recirculation affects both mixing and chemical timescales so that conceptually these burners are different from JHC and Cabra flames, which act solely on the chemical timescale. Despite the reasonable number of studies in the literature [15], the amount of detailed experimental data available for combustors operating under MILD/Flameless conditions is relatively scarce and limited to few operating

conditions. Based on such considerations, we report some results related to MILD combustion in a novel cyclonic burner [16]. Experiments have been performed in a propane-fired small-scale combustor and include detailed measurements of local mean temperatures. Experimental measurements in terms of temperatures were compared with detailed results of numerical computations in this configuration. This was done for a specific inlet temperature with a fixed mixture composition value. The main aim of the comparison between experimental and numerical data is to assess the considered modeling approaches to understand which method is more useful for prediction/design of MILD burners or which of them needs further modification/tuning.

The cyclonic combustion chamber

Experimental tests were conducted in a lab-scale cyclonic flow reactor. Fig. 1 shows a sketch of the section (a) and the front view (b) of the non-premixed configuration used to investigate the MILD combustion process [16]. It is a prismatic chamber with a square section of 0.2x0.2 m^2 and height of 0.05 m. The burner is fed with two pairs of coaxial oxidant/fuel jets. They are placed in an anti-symmetric configuration thus realizing a centripetal cyclonic flow field with a top-central gas outlet. The main oxidizer flow (N_2/O_2 mixture) is preheated at different temperatures and injected at 38 m/s whereas the fuel stream (N_2/C_3H_8 mixture) is settled at an environmental temperature (T_0=300 K) and 50 m/s. The oxidant injector is located at 0.02 m from the lateral wall and has a diameter of 0.008 m, whereas the fuel injector is at 0.045 m from the wall and has a diameter of 0.0008 m. The feeding configuration is shown in Fig. 1a. The gas exit is located on the top of the chamber.

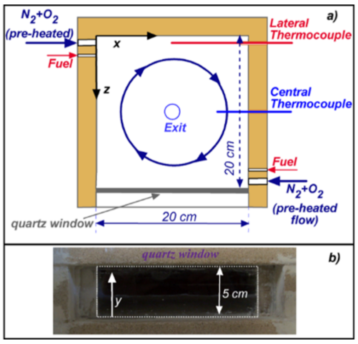

Figure 1. Sketch of the mid-plane section (a) and front view (b) of the cyclonic configuration

The combustor is built using a heat-insulating material (expanded vermiculite) and it is located within an electrically heated ceramic oven. The burner is equipped with two thermocouples (type N) and an optical access (a quartz window) as shown in Fig. 1. The thermocouples are located at the mid-plane and can be moved across the reactor. The lateral one is placed near the wall (at 0.02 m from the wall) while the central one is placed at the centerline of the combustion chamber (0.1 m from the wall) as depicted in Figure 1a. The uncertainties in the measurements are linked to convective and radiative effects and are ±2% and ±6% in the lateral side and ±1% and ±1.5% for the central one. Further details on the experimental apparatus can be found in previous literature works [17].

Numerical methodology

RANS simulations were carried out with the commercial code Fluent 17.0 by Ansys Inc. The grid was generated with the software Ansys ICEM. The first approach has been a full-hexa mesh. Several attempts with different cells numbers ranging from 400 k to 800 k have been made to test the structured approach. Despite the quite simple chamber's geometry, the structured mesh presented different convergence problems (large fluctuations of residual values and variables instability). It was therefore decided to opt for a polyhedral grid of 200 k cells. A grid independence study was performed using polyhedral grid with a number of cells ranging from 100 k to 400 k. The chosen grid consisted of 200 k polyhedral elements, generated from a 1200 k tetrahedral grid. Reynolds stresses were solved through the RNG k-ε turbulence model with swirl dominated flow corrections to account for the high swirl in the combustor. For turbulence-chemistry interaction, EDC (C_τ=0.4083-1.5) and PaSR were adopted. The mixing time scale of the latter was defined, following Ferrarotti et al. [12], as:

$$\tau_{mix} = C_{mix}\frac{k}{\varepsilon}, \tag{1}$$

where C_{mix} is a mixing constant defined here as 0.1 or 0.01. Instead, the chemical time scale was derived from approximating the Jacobian diagonal terms.
The Discrete Ordinate (DO) radiation model was used, while the radiation properties of the reacting mixture are considered with the Weighted-Sum-of-Grey-Gases (WSGG) model, by using the coefficients proposed by Smith et al. [18]. The GRI 3.0 (35 species, 217 reactions) [19] was used as kinetic scheme. On the other hand, was also assessed the capability of the combustion paradigms based on flamelet-like (FGM) for predicting MILD regime. FGM is a chemistry reduction method, which is based on two assumptions: a n-dimensional composition space can be represented by a lower dimensional manifold; and a turbulent flame is an ensemble of laminar flames [7, 20]. The inclusion of turbulence was made with a presumed $\beta - PDF$ approach. More information about the boundary conditions can be found in [20].

Results and conclusions

The stoichiometric case ($\phi = 1$) was investigated and evaluated numerically with the objective of comparing different combustion model formulations.

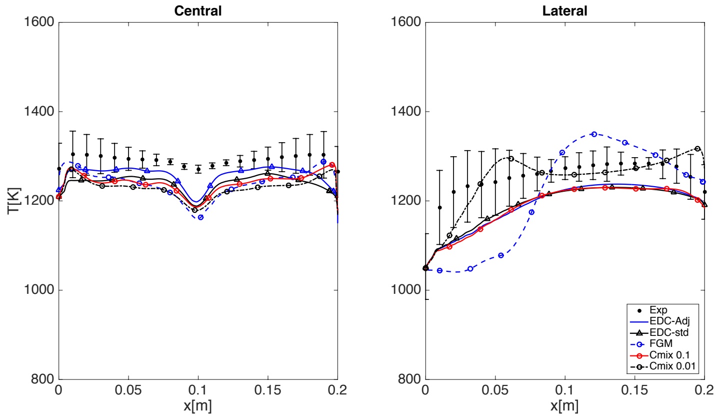

Figure 2. Axial profiles of the measured and predicted temperature profiles with different combustion model (Central and Lateral thermocouples).

All the models provide a satisfactory closure of the energy balance, since the exhausts and wall temperatures are in good agreement with the experimental ones. Differently from FGM, the EDC and PaSR predicted temperatures show a monotone behavior more similar to the experiments. Indeed, the small increase of temperature along the axial direction is well predicted, especially with PaSR-C_{mix}=0.01. Along the central thermocouple, all the models show a slight under-prediction in the proximity of the center of the burner on the order of maximum 6 % (for FGM). EDC-C_{τ}=1.5 is the model that best predict the lateral sides of the temperature profile.
All the model depicted some disagreements with respect to experimental data, therefore it will be very important to identify the failure of each model to improve them with respect to the combustion regime.

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