Optimization of FGM model for Mild Combustion in a cyclonic burner

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Introduction

The development of thermal efficiency with fuel flexibility and ultra-low emissions is one of the most challenging subjects for combustion researchers. Among the modern technologies developed for this challenge, MILD combustion [1] seems to be one of the most promising. It is a combustion regime characterized by fuel oxidation in an environment with relatively low oxygen concentrations and high inlet temperatures. 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, very low NOx and CO emissions and ensures large fuel flexibility, representing an ideal technology for low-calorific value fuels [2]. This combustion mode is achieved through the strong burnt gases and heat recirculation, which is obtained through special designs of the feeding jets as well as of the combustion chamber. Despite the reasonable number of studies in the literature [3], the amount of detailed experimental data available for combustors operating under MILD/Flameless conditions is relatively scarce. In recent years, attention has been paid to MILD combustion modeling, due to its very strong coupling between turbulence and chemistry. The flue gases entrainment, indeed, increases the initial inert content of the fresh mixture and kinetics time scales become comparable to the mixing ones so that the turbulence/chemistry interaction needs to be considered with an appropriate turbulent combustion model [4]. Attractive strategies for including detailed chemistry effects using moderate CPU resources are tabulated chemistry techniques. Among them, there is the Flamelet Generated Manifold (FGM) [5], which is based on flamelet assumption [6]. So, we report a study of characterization of MILD combustion in a novel cyclonic burner [7] using the FGM model.

The cyclonic combustion chamber

Experimental tests were conducted in a laboratory-scale cyclonic flow reactor. To the left of Fig. 1 a sketch of the section (a) and the front view (b) of the laboratory-scale burner used to investigate the MILD combustion process [7, 8] is reported. The burner is a prismatic chamber with a square section (0.2x0.2 m²) and height of 0.05 m. It 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 is preheated at different preheating levels (T_in) whereas the fuel stream is propane at environmental temperature (T_0). The oxidant injector is located at 0.02 m from

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the lateral wall, whereas the fuel injector is at 0.045 m. The feeding configuration is shown in Fig. 1a. The gas exit is located on the top of the chamber.

![Diagram showing the midplane section and front view of the cyclonic configuration](image)

**Fig. 1** Sketch of the midplane section (a) and front view (b) of the cyclonic configuration to the left; list of the conditions investigated to the right.

<table>
<thead>
<tr>
<th>RUN</th>
<th>$T_0$ (K)</th>
<th>$T_{in}$ (K)</th>
<th>$\Phi$</th>
<th>$d$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CL1045</td>
<td>300</td>
<td>1045</td>
<td>0.33</td>
<td>0.94</td>
</tr>
<tr>
<td>CS1045</td>
<td>300</td>
<td>1045</td>
<td>1</td>
<td>0.94</td>
</tr>
<tr>
<td>CR1045</td>
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<td>1045</td>
<td>1.67</td>
<td>0.94</td>
</tr>
<tr>
<td>CS1075</td>
<td>300</td>
<td>1075</td>
<td>1</td>
<td>0.94</td>
</tr>
<tr>
<td>CS1125</td>
<td>300</td>
<td>1125</td>
<td>1</td>
<td>0.94</td>
</tr>
</tbody>
</table>

The cyclonic burner is equipped with two thermocouples (type N) at the mid-plane and a quartz window as optical access (Fig. 1b). Two movable thermocouples are located at the mid-plane. The lateral one is placed 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). The exhausts were monitored at the exit and the major species emissions were analyzed by means of a GC analyzer. The full list of the experimental runs performed is summarized to the right of Fig. 2, where $d$ is the dilution level and $\Phi$ is the equivalence ratio.

**Methodology and numerical setup**

Numerical simulations were performed with the commercial code ANSYS Fluent. The complete 3D geometry and the computational grid were realized using the software ANSYS ICEM. The mesh used is composed of 411064 hexahedral elements, clustered near the inlets. Favre-averaged Navier–Stokes equations were solved using RNG k-ε turbulence model with swirl dominated flow corrections to account for high swirl in the combustor. As mentioned, in this study is 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. The lower dimensional manifold can be constructed by solving a one-dimensional flame and tabulating the related quantities as functions of a few controlling variables (CVs). During a CFD simulation, only the transport equations for CVs are solved and the required variables are looked-up from the so-called FGM look-up tables. Following the study from Sabia et al. [9], C1C3 reaction mechanism [10] was used. As 1D flame type to be computed in the flamelet solver Chem1D [11], the Igniting Mixing Layer (IML) approach [12] was chosen. In this configuration fuel and oxidizer are initially placed side-by-side and then mix by molecular diffusion and react in time. First, an adiabatic table with only two CVs (100x100 points) were built: A Progress Variable (PV), defined as a combination of the mass fractions of H$_2$O, CO$_2$ and HO$_2$; and a mixture fraction (Z), computed using Bilger’s formula, to represent the molecular mixing between fuel and oxidizer. Afterwards, a non-adiabatic
table was built including the total enthalpy as additional CV (100x100x15 points). To do that, flamelets at lower enthalpy content were calculated decreasing the oxidizer inlet temperature. So, 2D laminar and adiabatic tables were created for each condition reported in Fig.1 while a 3D laminar and non-adiabatic table was constructed only for the condition CS1045. For turbulence-chemistry interaction, a presumed β-PDF approach was adopted. Regarding adiabatic tables, a 4D turbulent table was created using built-in FGM option in Fluent with 101x101x11x11 points in the means and variances of CVs and a total of four transport equations were solved including the heat loss in the CFD runs. Afterwards, for the non-adiabatic table, a 5D turbulent table was built adding 15 enthalpy points. The table was created by in-house codes and stored by means a User Defined Function in Fluent, where a total of five transport equations were solved.

Results

The numerical computations were performed incorporating FGM to the RANS simulations. Experimental tests and numerical runs were carried out for C3H8/O2/N2 mixtures, at environmental pressure and mean residence time of 0.5 s for the conditions reported to the right of Fig. 1. In Fig. 2 the results for the adiabatic tables of temperature distributions and species concentration at the exit varying Φ at Tin=1045 K, are presented.

![Fig. 2](image)

In this case, experimental and FGM results depict slightly good agreement both for temperature trends, especially downstream and in the central part of the burner, and for the overall species production. However, there are still some discrepancies to be addressed. Firstly, the temperature close to the oxidizer nozzle exit is under-predicted by the numerical model. This could be related to the burned gas recirculation inside the chamber, to the adiabaticity of the tables and to neglecting the radiation effects from and to the walls. Another slight disagreement is observed in the prediction of the mole fractions of species like H2 and CO. In order to take into account the non-adiabaticity effects, a comparison between enthalpy-not-included and enthalpy-included tables is reported in Fig. 3, for the case CS1045. It is possible to notice that, including the total enthalpy as CV, the prediction of the temperature axial profiles improves: there is a better agreement near the nozzle, where the temperature is still under-predicted but the ignition is earlier; and in the central part the temperature profile is more homogeneous.
Fig. 3 Measured and predicted temperature axial profiles and species concentration at outlet for the case CS1045.

On the other hand, the prediction of the molar concentration of the main species at outlet gets worse for the 5D table, especially for the hydrocarbon species. This suggests that the conditions looked up from the table correspond to partially burned ones.

Conclusion

The three main objectives of this work are: assess the performance of FGM with IML configuration and evaluate the adequacy of the kinetic mechanism; examine the effects of the operating parameters such as $T_\text{in}$ and $\Phi$ on the predictions; define the importance of including enthalpy as CV for this kind of burner. The numerical results demonstrated that FGM with IML is a promising tool for modeling the complex flame structures of the cyclonic MILD burner. Aspects like the inclusion/replacement of CVs in the manifold, usage of a different canonical reactor type and the inclusion of a reliable radiation model, will be considered in the future. Finally, the preliminary 5D table results will be extended for all the experimental conditions to improve the validation.

References