Reaction-rate based modeling of MILD Combustion in a cyclonic burner

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Abstract
MILD combustion is a regime in which oxidation reactions occur without a deflagrative flame front. CFD plays a key role in the successful introduction of such a concept for several industrial applications. In this framework, this work aims to improve the knowledge about the modeling requirements of such a regime in a scale-bridging burner, which ensures MILD combustion condition through an internal recirculation of flue gases and thus mimics industrial devices. Different dilution conditions are simulated through reactive FANS simulations, by implementing modifications proposed in literature of the Eddy Dissipation Concept model for the treatment of the turbulence-chemistry interaction.

Introduction

Novel combustion concepts are intensively investigated in recent decades as a consequence of new scenarios regarding the energy mix and diversification of sources. Among them, Moderate or Intense Low-oxygen Dilution (MILD) Combustion, has been recognized as a promising technique to increase thermal efficiency, reduce the pollutant emissions and operate with a wide palette of fuel in a single combustion unit [1]. Such oxidation mode exhibits similar features to other technologies such as Flameless Oxidation (FLOX) [2], High Temperature Air Combustion (HiTAC) [3] or Colorless Distributed Combustion (CDC) [4].

To ensure MILD combustion, the inlet preheating level of the reactant mixture should be higher than the self-ignition temperature, while the maximum allowable temperature increment should be lower than T_{ign} [5]. The corresponding operative conditions are usually achieved through internal or external exhaust gas recirculation (EGR) methods [6][7]. To ensure proper recirculation levels, a proper design of the chamber and position of the inlets is needed. Indeed, a possible method to trigger internal recirculation is the use of of high-momentum jets at the inlets [8].

Several configurations mimic MILD combustion through a fuel jet within a hot and diluted coflow to promote reaction that occurs in the shear layer between the two streams. Examples are the Cabra flame [9] and Jet-in-Hot-Coflow (JHC) burners from Adelaide [10] and Delft [11]. In such flames, low-oxygen conditions are locally achieved acting on the chemical time-scale; the stabilization of the flames is ensured by means of bluff-body or swirl flow and the combustion typically occurs far from the walls.

Besides, in technological applications of such a concept, the large-scale recirculation of flue gases has a key role in providing locally the desired dilution levels before the occurrence of ignition. Therefore, the local oxygen content significantly influences both the mixing and kinetics time scales, making such systems highly different from Jet-in-Hot-Coflow flames. Moreover, in the latter configurations, the flameless characteristics are very difficult to be identified due to the absence of the walls and therefore the homogeneity of the thermal field and low species gradients usually observed in furnace-like with strong EGR configurations are not recognized in unconfined flames [12]. Differently from Jet-in-Hot-Coflow flames, in several MILD configurations, due to the long residence times and the flow confinement, the heat transfer at walls has a key role and thus the reactive region is stabilized far from adiabatic conditions [13][14]. In such oxidative conditions the chemistry and mixing time scales are comparable and, thus, the Damköhler number is very low, reaching values close to unity [15]. Galletti et al. [16] analyzed both the turbulence and chemical timescales and confirmed that the high-temperature region in MILD is characterized by Damköhler numbers lower than those observed in conventional flame mode. Recently, Zhang et al. [17] numerically evaluated the influence of the injection parameters on the Damköhler number, showing that its reduction is crucial in establishing the MILD regime. Recently, Swaminathan [18] obtained through several Direct Numerical Simulations (DNS) physical insights on the MILD combustion regime. He concluded that the fundamental aspects of this oxidation mode are still not well-understood, especially concerning the typical morphological and topological features of the reaction zones. However, the observations derived from DNS studies shed some light on the reaction zone modeling in MILD modes. Specifically, reaction-rate based modeling could represent a viable approach for MILD combustion [19]. Such studies also suggested that there is room for improvement of the Eddy Dissipation Concept (EDC) for treating the turbulence-chemistry interaction, by accounting for changes in the local reaction zone volumes, considering the effect of dilution on characteristic scales [20].

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In this context, the present work describes the implementation of the EDC model to incorporate finite rate kinetics at affordable computational cost, when simulating a lab-scale MILD burner. The commonly used EDC model is revisited according to the modification proposed in the literature for MILD combustion. Its applicability is validated with data obtained on a cyclonic combustion chamber with several feeding conditions.

Experimental setup

The Laboratory Unit Cyclonic Burner (LUCY) used in this work is illustrated in Figure 1 and is described in several literature papers [21][22]; thus, only the main features will be recalled here. It presents a square section of 0.04 m^2 and a height of 0.05 m. Due to the position of the exit on the top-center of the chamber, a cyclonic flow field is stabilized by means of two couples of coaxial oxidant/fuel inlet jets placed in an anti-symmetric configuration. Two movable N-thermocouples are located inside the burner to monitor the temperature on the mid-plane of the chamber. The major pollutants such as CO, NOx and unburned hydrocarbons are monitored at the exit through gas analyzers.

The present experimental campaigns were carried out with a thermal power P = 2 kW by feeding methane with a fuel-air equivalence ratio $\phi = 1$ and different dilution levels, d (see Table 1) with:

$$d = \frac{mol_{N2}}{mol_{N2} + mol_{O2} + mol_{CH4}}$$

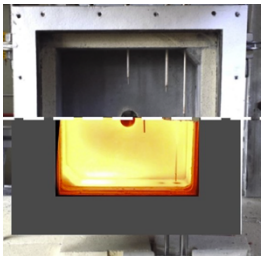


Figure 1- Picture of LUCY.

Table 1 – Experimental conditions and predicted recirculation factor.

case	d [%]	$\dot{m}_{CH4}$ [kg/hr]	T_{CH4} [K]	$\dot{m}_{N2+O2}$ [kg/hr]	T_{N2+O2} [K]	T_{flue} [K]	k_v [-]
D71A	71.5	0.123	300	2.16	1000	1270	6.5
D80	80	0.123	300	3.16	1000	1255	7.5
D90	90	0.123	300	6.48	1000	1211	8

Numerical model

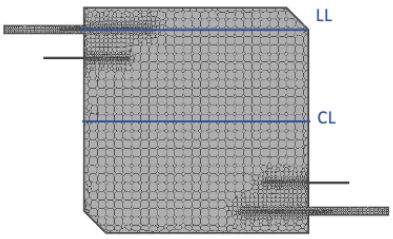
Favre-averaged Navier-Stokes (FANS) equations for continuity, momentum, energy, and transport of chemical species are solved in steady conditions by using the coupled solver available in Fluent by ANSYS Inc., based on the finite volume method. The Reynolds stress tensor is closed through the Re-Normalization Group (RNG) $k-\varepsilon$ model. Preliminary, the Shear Stress Transport $k-\omega$ model and the Reynold Stress Model were also tested; however, they showed larger discrepancies with the experimental data than the RNG $k-\varepsilon$ model.

The turbulence-chemistry interaction is handled in different manners, i.e., with: the standard EDC; the EDC with an increased value of the constant for the residence time in the fine structures, i.e., C_τ (see [23] and [24]) and EDC with modification of [25]. According to the latter model, the coefficients for the fine-structure mass fraction and residence time, i.e., C_γ and C_τ, respectively, are expressed as a function of the local Reynolds and Damköhler number. The model is implemented in the CFD code through a User Defined Function (UDF).

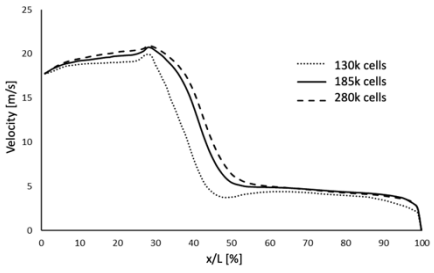
The KEE-58 with 17 chemical species and 58 reversible reactions [26] is employed to describe oxidation, as successfully applied in several works dealing with MILD combustion [27]. Radiation is modeled with the Discrete Ordinate Model by using the Weighted Sum of Grey Gases (WSGG) to estimate the spectral properties of the gas medium.

Boundary conditions consisted of uniform velocity, temperature and composition at the inlets, no slip condition and negative heat flux to account for dispersion at the wall and pressure outlet at the chamber exit.

The computational grid is made of polyhedrons with prism layers at the wall to better control the $y+$, which was kept <1. Details on the grid refinements near the injection nozzles are reported in Figure 2a. A grid independency study was preliminary carried out in non-reactive conditions by using 3 computational grids with a number of cells between 130k and 280 k. The velocity profiles along the lateral line, i.e., LL, predicted with the three grids are reported in Figure 2b; consistently the medium-sized grid with 185k cells was adopted.



(a)



(b)

Figure 2 - Computational grid (a) and velocity profiles predicted with 3 different computational grids along the lateral line, i.e. LL (b).

The second order upwind interpolation was adopted for the spatial discretization, while the Semi-Implicit Method for Pressure-Linked Equations (SIMPLE) allowed to take into account for the pressure-velocity coupling.

Numerical Results

The fluid dynamics, which is triggered by the position of the inlet jets, is shown through flow streamlines, colored by the residence time, in Figure 3. The internal recirculation degree can be estimated as the ratio between the internal recirculation flow rate, i.e., $\dot{m}_{TOT}$, and the whole flow rate entering the chamber as:

$$k_v = \frac{\dot{m}_{TOT}}{\dot{m}_{CH4} + \dot{m}_{N2+O2}}$$

Here, $\dot{m}_{TOT}$ is estimated from the numerical predictions by integrating the tangential velocity in the half vertical mid-plane of the combustion chamber. The resulting k_v values are reported in the last column of Table 1 for the three dilution cases.

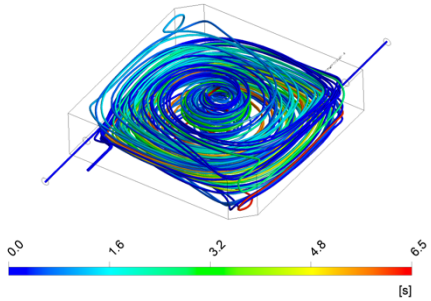


Figure 3 - Flow streamlines colored by residence time.

The temperature fields in the horizontal mid-plane of LUCY, predicted with the different EDC formulations are shown in Figure 4a,c,e for the reference case, i.e., D71a, while the comparison with experimental data is provided in Figure 5. It is worth recalling that the EDC modifications suggested in the literature [23][24][25] are all based on JHC configurations, which achieve MILD combustion through a fictitious dilution of the oxidant stream. The JHC is hence much different from LUCY, which, instead, ensures MILD combustion with an internal recirculation, thus mimicking industrial furnaces and ovens. From the perspective of the turbulence-chemistry interaction, the JHC configuration acts solely on the chemical time-scale, while LUCY affects both chemical and turbulent time-scales.

The increase of the residence-time constants in the fine structure from the default value, i.e., $C_\tau = 0.41$, to $C_\tau = 1.5$ [23] or $C_\tau = 3.0$ [24] hampers reactions too much, so that the flame is unable to ignite. Hence, a preliminary sensitivity analysis on C_τ was carried out and a value of $C_\tau = 0.8$ was chosen. The corresponding thermal and OH fields in the horizontal mid-plane are illustrated in in Figure 4c,d. We observe a strong impact of C_τ on the results, as there are significant differences with respect to the original EDC.

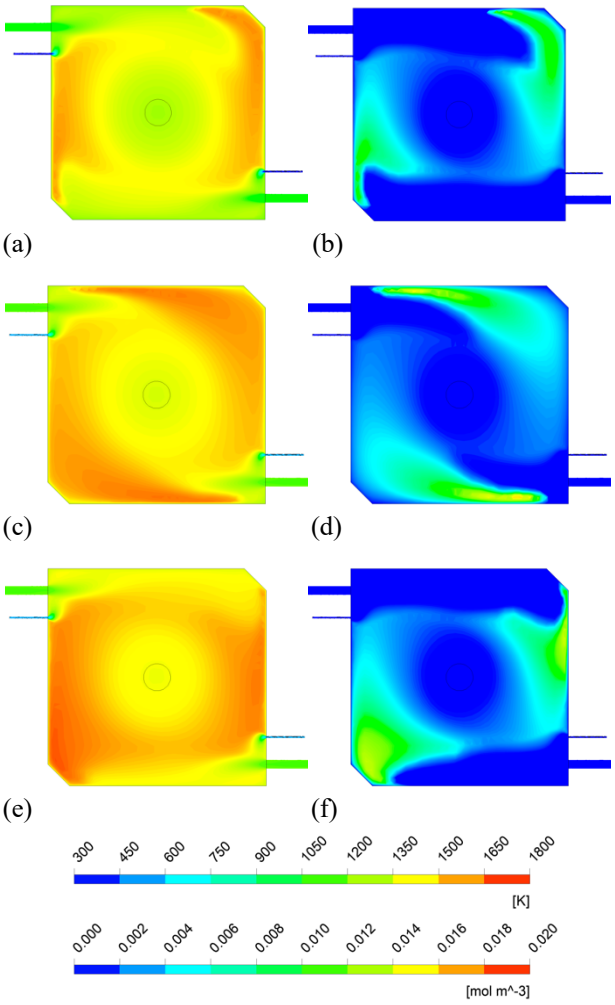


Figure 4 - Temperature (a,c,e) and OH concentration (b,d,f) for the D71a case and: (a,b) standard EDC; (c,d) EDC with C_t =0.8 and (e,f) EDC with UDF. D71a case.

As for the EDC from Parente et al. [25], the numerical simulations indicate a loss of the point-wise symmetry of the fields that we imagine from the geometry of LUCY. This unexpected behavior is especially evident from the reaction region marked with OH in Figure 4f and requires further investigation.

The comparison with the experimental data is reported in Figure 5a and Figure 5b for the central and lateral lines, i.e., CL and LL (see Figure 2), respectively. Along the CL, all models overestimate the temperature near the walls, while they underpredict the temperature near the center. The models with standard and $C_\tau = 0.8$ EDC, perform similarly near the CL center, while laterally we observe that the increase of the fine-structure residence-time constant limits the temperature peaks. Along the LL, all models predict a slower temperature rise than the measured one. This may be partly imputed to the deficiency of the FANS approach in well predicting the mixing of the inlet jets. Similar behaviors were also observed especially along the lateral position when tabulated chemistry with β-pdf methods were employed for the turbulence-chemistry interaction description [22].

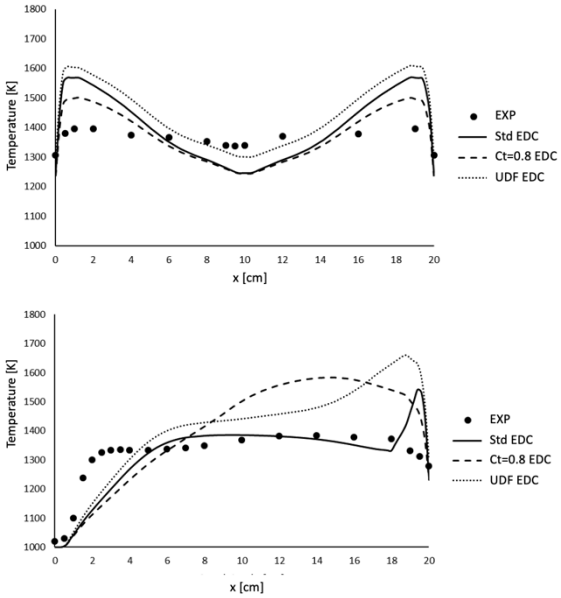


Figure 5 - Comparison between experimental temperatures along the CL (a) and LL (b) lines and those predicted by the 3 EDC formulations. D71a case.

At larger distances from the entrances, both the two EDC modifications lead to a strong overprediction of temperature. Instead, the standard EDC is better in agreement with the experimental data, except for the presence of a temperature peak near the walls which is not captured in the experimental campaigns.

For these reasons, the standard EDC will be used for the other cases, i.e. D80 and D90. The effect of dilution on the resulting temperature and OH distribution on the burner horizontal mid-plane is shown in Figure 6. We notice how increasing *d*, the temperature peaks smooth resulting in more uniform fields. The reaction zone, which can be located in the green regions of the D71a and D80 cases (i.e., Figure 6b and Figure 6d, respectively) is well distributed for the D90 case (see Figure 6f).

The comparison with the experimental temperature measurements is provided in Figure 7 and Figure 8 for the CL and LL, respectively. For a better comparison, the experimental and numerical error bars are reported. The latter bars were estimated from the temperature variance due to jet fluctuations and radiation uncertainties. We observe how increasing the dilution, both numerical and experimental temperature profiles on the CL (see Figure 7), flatten. The over-prediction of temperature near the wall diminishes with increasing the dilution, with satisfactory agreement between experiments and numerical results for D90. The temperatures near the center are generally well captured for both D80 and D90.

For the lateral line (see Figure 8) we observe that the numerical predictions underestimate the temperature rise near the injection also for the D80 case, while a good agreement is found for the D90 case. The numerical results of the D80 case shows a temperature peak near the wall, like the one observed for D71, which is not measured experimentally. Instead, such peak is not present for the D90 case. Such case, with the highest dilution levels, is the one that show the better agreement between experimental and numerical predictions.

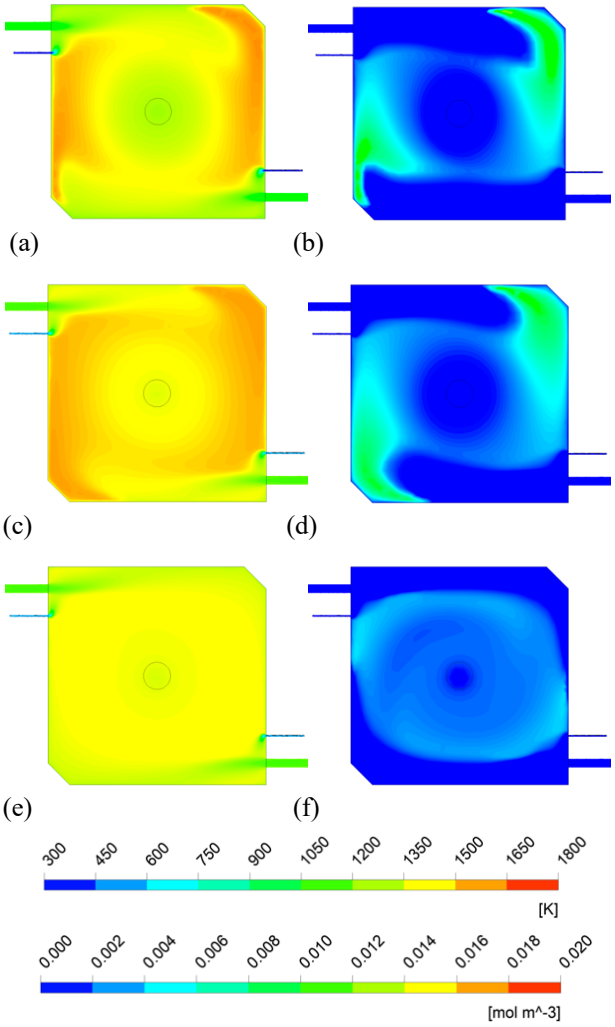


Figure 6 - Temperature (a,c,e) and OH concentration (b,d,f) predicted with the standard EDC for different dilution levels: (a) D71a; (b) D80 and (c) D90 cases.

Previous works reported similar behaviors especially when referred to the lateral position also when primitive-variable approaches are used [22].

Thus, both the reaction-rate and tabulated chemistry models seems to be able to predict very well the system reactivity for “MILD external conditions”, i.e. for high inlet dilution levels. On the other hand, for “MILD internal conditions” with low inlet dilution, the model cannot account for the impact of the internal dilution on the reactivity and, therefore, both the methods overpredicts the experimental data at the inlet zone, where ignition occurs.

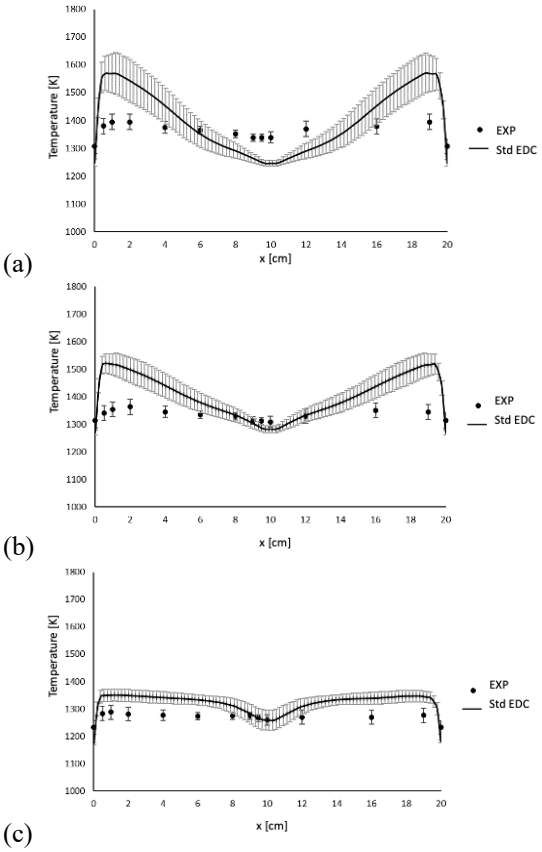


Figure 7 - Comparison between experimental and predicted temperatures along CL for different dilution levels: (a) D71a; (b) D80 and (c) D90 cases.

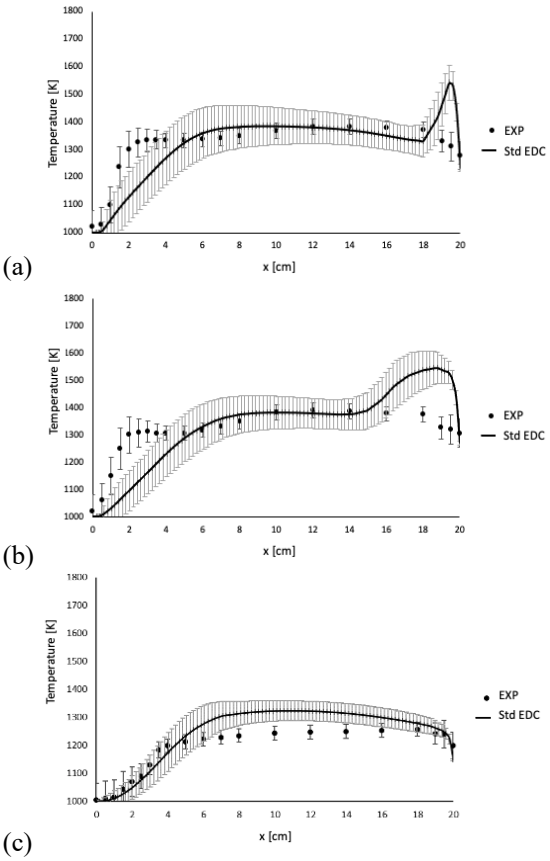


Figure 8 - Comparison between experimental and predicted temperatures along LL for different dilution levels, i.e: (a) D71a; (b) D80 and (c) D90 cases.

Conclusions

Different modifications of the Eddy Dissipation Concept suggested in the literature for treating the turbulence-chemistry interaction in MILD combustion conditions are implemented for the numerical simulations of a lab-scale burner which achieves distributed combustion conditions through a strong internal recirculation. The system is especially interesting as it emulates industrial furnaces operated with internal recirculation.

Conceptually, the low Damköhler numbers needed for MILD conditions are achieved by both increasing the chemical time-scales, due to the dilution of reactants, and reducing the flow time-scales due to the intense recirculation. This feature differs strongly from that of the Jet-in-Hot-Coflow flames for which EDC modifications have been proposed. Indeed, in such flames, MIDL combustion is achieved by acting solely on the chemical time-scale.

The EDC modifications were found to be not effective in improving the numerical predictions. In particular, the increase of the residence time constant of EDC up to the values proposed in the literature, dampens the reactions too much, preventing ignition.

The comparison between numerical predictions and experimental in-flame data showed a good agreement for the highest dilution case, i.e., D90. However significant discrepancies were observed for the D71a and D80 cases that deserve further investigation.

In particular, the experimental temperature profiles along the central line are generally flatter than the predicted ones; this may suggest also a revision of the heat transfer model for instance of the WSGG for estimating spectral properties. The temperature profiles along the lateral line show that the numerical model generally underpredicts the heating rate of the oxidant jet suggesting to need to improve the prediction of its mixing.

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