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STSM Title: Modeling of MILD Combustion in a cyclonic burner with Flamelet-Generated-Manifold (FGM) model

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Background/ Purpose of the STSM

Reducing pollutant emissions, increasing the fuel flexibility and improving burners efficiency has brought to the development of new combustion concepts. Among these new technologies, MILD combustion seems to be one of the most promising. This 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 and very low NOx and CO emissions. In MILD combustion, the inlet temperature of the reactants is higher than the auto-ignition temperature of the mixture and, simultaneously, the maximum temperature increase due to oxidation reactions remains lower than the mixture auto-ignition temperature because of high dilution levels.

Although MILD combustion systems have been successfully introduced in some industries, broad implementation is hampered by a lack of fundamental insight into this combustion regime.

Moreover, MILD combustion burners and furnaces often show a complex geometry designed to improve the reactant dilution through internal recirculation of flue gases, so that the derivation of simple conceptual models is difficult. In such cases, the use of CFD tools for understanding the burner behaviour and for design optimization appears essential.

A key point necessary for efficient design of a MILD combustor is to ensure good mixing between the incoming fresh fuel/air mixture and the hot burnt gases. This can be achieved by designing combustor aerodynamics with strong recirculation that redirects the hot products towards the injection nozzle. Another difference is that the reaction dynamics are governed by stirring controlled processes since fresh gases have to mix with burnt products prior to ignition and reaction. Consequently, the simulation tools should include accurate models for describing both turbulent stirring/mixing and chemical reactions.

MILD combustion modeling requires different tools compared to traditional combustion simulation.

Attractive strategies for including detailed chemistry effects using moderate CPU resources are tabulated chemistry techniques. Among such models are flamelet generated manifold (FGM) techniques, which are based on flamelet assumption. They have been applied to MILD combustion successfully.

FGM is a chemistry reduction method, which is based on two assumptions: 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 (CV). During a CFD simulation, only the transport equations for CV are solved and the required variables are looked-up from the so-called FGM tables. Important selections to be made in an FGM study are the determination of CV and the type of 1D flame to be solved. In non-premixed combustion, the traditional approach is to use mixture fraction (Z) and a reaction progress variable (PV) as CV, and to select PV as combination of products and/or reactants mass fractions. It was shown in engine related studies that addition of precursors to the classical definition of PV is required to capture the autoignition. As for the 1D flame type, although the common practice is to use counter-flow (CF) type flames, Abtahizadeh et al. showed that igniting mixing layers (IML) type flame is a better option in representing MILD combustion in a jet in hot coflow (JHC) burner.
The elucidation of the above topics needs high fidelity and comprehensive experimental data to validate the numerical models. JHC setups from Adelaide, and Delft, and the Cabra flame have been conceived to emulate flameless conditions by feeding diluted and hot streams to the burner. They constitute a strong asset for the validation of numerical models as they have been equipped with advanced diagnostics to measure mean and fluctuating variables (e.g. chemical species, temperature, velocities).
However, in the industrial practice, MILD Combustion conditions are obtained by means of the massive internal recirculation of flue gases, which allows diluting the fresh gases before they reach the reaction zone. Such recirculation is generally achieved through special designs of the feeding jets as well as of the combustion chamber.
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, the amount of detailed experimental data available for combustors operating under flameless conditions is relatively scarce and, in general, when reported, is for very few and narrow combustor operating conditions. Therefore it is important to extent the present database on MILD Combustion and thereby to improve the understanding of the processes which occur during this combustion regime. To this end, the combustion process in a cyclonic burner that operates in MILD combustion conditions was investigated experimentally and the main purpose of this STSM is to use RANS simulations with FGM sub-model in order to prove and validate the capability of the numerical model to represent the underlying physics of this combustion regime in the present combustion chamber.

Description of the work carried out during the STSM

The first days of the STSM were dedicated to gaining experience on how to set up the case for tuning and calibration of initial conditions to match the experimental conditions. In particular Fluent software was used with User-Defined-Function in order to implement the look-up table that was generated by means of CHEM1D.

An important part of an FGM simulation is to select an appropriate 1D flame type to be used in table generation. Counter-flow (CF) configuration is a commonly used one, where two opposing jets are issued on to each other and the flame develops at the stagnation plane. However, the igniting mixing layer (IML) approach is used, where the fuel and oxidizer are placed side-by-side initially, they mix by molecular diffusion, and react in time. Evolution of temperature in a sample IML simulation is shown in Fig. 1.

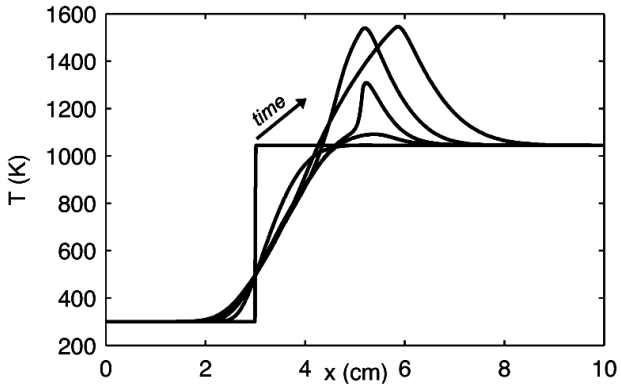

Fig. 1 Evolution of temperature profile for a sample IML case

Since the structure of co-flowing inlet jets in the present burner is similar to IML, it is selected as the 1D flame type in this study. It can be argued that the use of homogeneous reactors would be a better option considering the uniform flame structure in MILD combustion. However, the pre-ignition chemistry takes place as the jets start to mix and this cannot be captured with 0D models.

Progress variable (PV) was selected as a combination of Y_{H2O}, Y_{CO2} and $Y_{HO2.}$ Mixture fraction (Z) computed using Bilger's formula was used as the second CV to represent the molecular mixing between the fuel and oxidizer. Although there is heat loss from the burner to the surroundings, this was not accounted for in FGM table creation to limit the table dimension and thus reduce computational needs.

In the CFD simulations, ANSYS Fluent was used as the solver. RANS equations were solved using RNG k-ε turbulence model with swirl dominated flow corrections to account for high swirl in the combustor. For turbulence-chemistry interaction, presumed β-PDF approach was adopted. A total of four transport equations for the means and variances of CVs were solved for the FGM part using built-in FGM option in ANSYS Fluent. A 4D FGM table was constructed using 101x101x11x11 points in the mean and variance of CVs, respectively.

Although heat loss was not used in manifold creation, it was included in the CFD runs. A heat transfer coefficient of 10 cal/(m^2 s K) and $T_{ambient}=T_{in}$ were prescribed at the walls as the thermal boundary condition. This way, the effect of heat loss could be reflected on the prediction of temperature and thermodynamic properties, but not on the reaction rates and heat release.

The computational mesh used is composed of 411064 hexahedral elements, clustered near the inlets. Velocity inlet BCs were used for the fuel and oxidizer jets, while pressure outlet BC was used for the outlet. Pressure-velocity coupling was ensured using SIMPLE scheme, and second order upwind discretization was used for all the transported variables.

The temperature slice from the mid plane and the surface mesh of the whole domain from the simulation with stoichiometric conditions and T_{in}=1045 K is given in Fig. 2 to provide an idea on how the simulations look like.

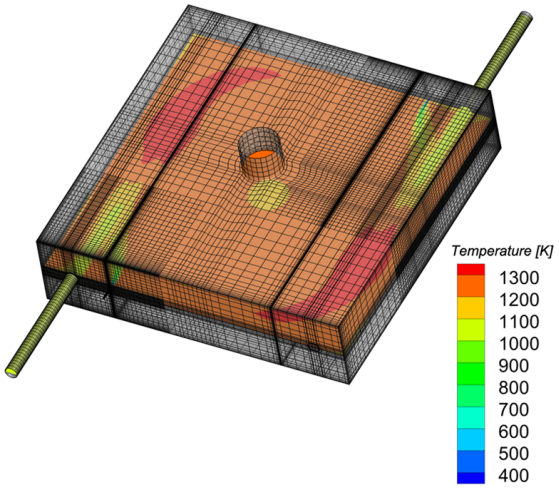

Fig. 2 Computational mesh and mid-plane temperature profile for a stoichiometric inlet condition

Numerical simulations were carried out for $C_3H_8/O_2/N_2$ mixtures, at environmental pressure and mean residence time of 0.5 s inside the combustor. The operating conditions were chosen in order to match the experimental ones. The external parameters such as the inlet temperatures of the main flow (Tin) and the overall equivalence ratio (Φ) at the inlet were varied parametrically in order to investigate the combustion behavior of the system. The overall external dilution level is kept constant at 94% for all the investigated conditions.

The results of the comparison between experimental and CFD analysis of the cyclonic burner are presented and discussed in the next section with two main objectives:

i) to assess the performance of the chosen tabulated chemistry model (FGM with IML configuration) and evaluate the adequacy of the kinetic mechanism

ii) to examine the effects of the operating parameters (Tin and Φ) on the temperature distributions and species emissions, as well as on the accuracy of the numerical predictions.

The full list of the simulated cases is summarized in Table 1

Table 1 List of the experimental conditions investigated in this study

RUN	***T_0 (K)***	***T_{in} (K)***	***Φ***	***Dilution level (d)***
CL1045	*300*	*1045*	*0.33*	*0.94*
CS1045	*300*	*1045*	*1*	*0.94*
CR1045	*300*	*1045*	*1.67*	*0.94*
CS1075	*300*	*1075*	*1*	*0.94*
CS1125	*300*	*1125*	*1*	*0.94*

Description of the main results obtained

The inlet mixture composition is a crucial parameter which affects the thermal field and the species production. To investigate these effects, the experimental results have been corroborated by the modeling activity. In the left column of Fig. 3 the axial temperature profiles obtained with the FGM-IML computations are reported with a black solid line for the three equivalence ratio values in order to compare and validate the model against the experimental data.

The small increase of temperature measured along the axial direction is reasonably well predicted when lean or fuel-rich inlet mixture compositions are used, although the temperature rise happens earlier in the experiments compared to the model. This is because the lateral thermocouple is positioned at the centerline of the oxidizer inlet, whereas the reactions start to occur between the fuel and oxidizer inlets in the simulations. There is a slight overshoot of temperature at the stoichiometric condition, which corresponds to the most reactive condition in the simulation.

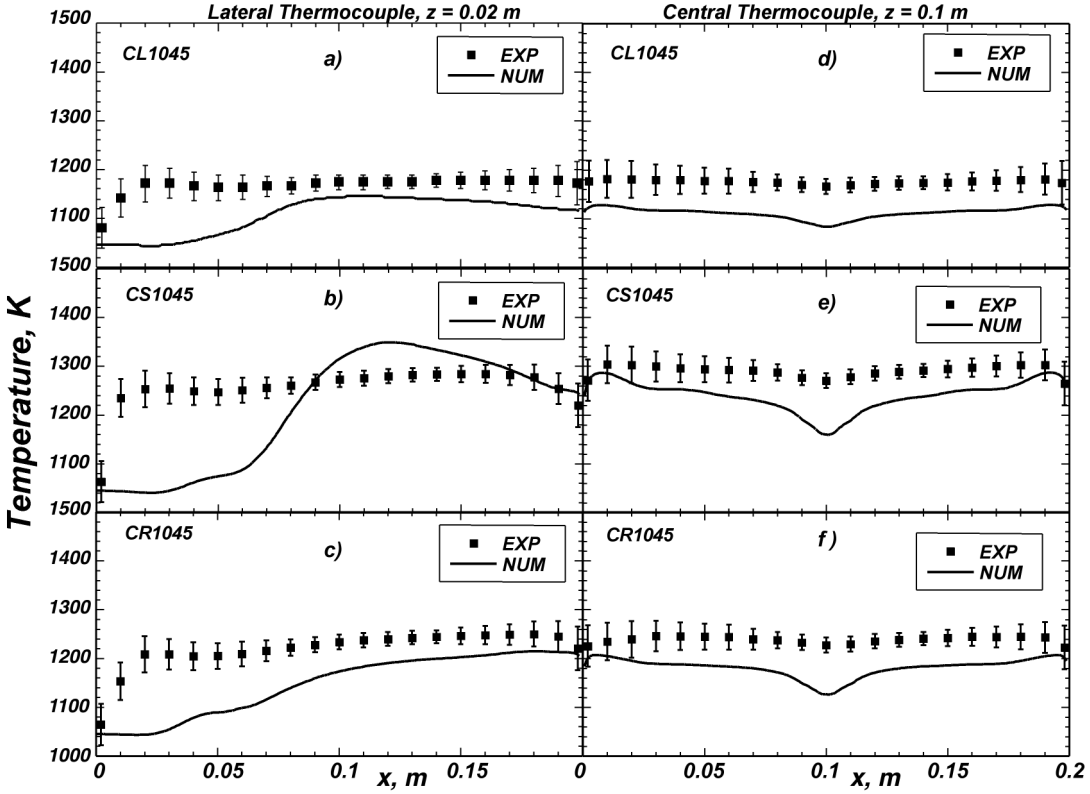

Fig. 3 Axial profiles of the measured and predicted temperature profiles parametric in the equivalence ratio (Lateral and Central thermocouples)

The simulated results show that the ignition starts between oxidizer and fuel jets thus partially explaining the slight underprediction of the model close to the nozzles. In fact the present tabulated model does not account for product gas dilution by means of internal recirculation. Previous works have emphasized the significance of dilution in the nonequilibrium chemistry and flame stabilization for internal recirculation systems but the addition of dilution parameter as another controlling variables implies higher table dimensions and CPU costs.

Axial profiles of temperature are reported in Fig. 3 (d-f) for the central thermocouple (z=0.1 m). The temperatures obtained with FGM are in very good agreement with measurements for all the cases and they show the same trend. In particular, in proximity of the center of the burner FGM results produce a slight underprediction on the order of maximum 6 % at stoichiometric conditions whereas it is lower for other conditions. Thus, the tabulated

combustion model selected reproduces very well the temperature distributions and homogeneity in such a system in the peripheral region where ignition has already occurred. Despite that the model underpredicts the temperature close to the nozzles and this is probably due to an overestimation of the heat exchange coefficient.

Moreover the effect of the inlet preheating level of the oxidizer jet was also investigated, as it is a key parameter for the occurring of MILD Combustion conditions.

The temperature field from the simulations are extracted and also shown in Fig. 4a. The model shows discrepancies for location close to the nozzles. This is again due to ignoring the effects of heat loss on the chemistry and it is also related to the heat loss overestimation.

On the other hand, the simulation results show a slight overprediction at 8<x<16 cm that increases with the Tin value.

The predicted temperatures, obtained with FGM and reported with the solid profiles in Fig. 4b are in very good agreement with measurements for all the cases and they show the same trend. In particular, in proximity of the center of the burner FGM-IML results reproduce a slight underprediction that is decreased for higher preheating level.

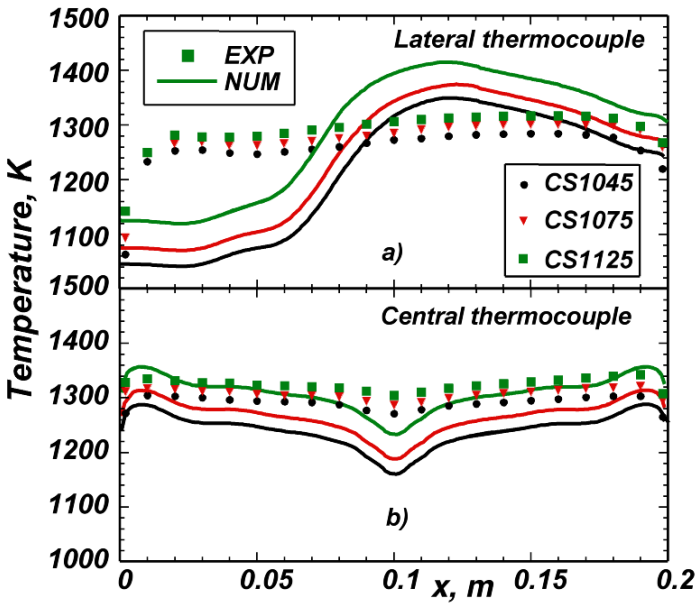

Fig.4 Temperature profiles parametric in Tin (Central and Lateral thermocouples)

The combustion process was investigated in detail by measuring the temperatures and emissions, and comparing them with those from the numerical model. Experimental and numerical results are quite good agreement and the numerical model is capable of predicting very similar trends of temperature and also the overall species production. However, there are still some discrepancies to be addressed. Firstly, the temperature close to the oxidizer nozzle exit is undepredicted by the numerical model. This can be attributed to the internal recirculation in the experiments, which cannot be exactly modeled by the current implementation due to lack of a dilution parameter in the manifold construction.

The numerical results of this work demonstrated that FGM with IML is a promising tool for modeling the complex flame structures of cyclonic MILD burner, with lots of room for improvement. Many aspects like inclusion of a dilution parameter and/or heat loss in the manifold generation, reevaluation of heat transfer coefficient at the walls, usage of a different chemistry mechanism and flamelet type will be considered in the future.

Future collaboration with host institution

The collaboration between the IRC-CNR in Naples and the Combustion technology group at the University of Eindhoven with regards to modelling of cyclonic combustor data using FGM model and CHEM1D software is established from a couple of years. Both institutions plans to maintain the ongoing collaboration that would lead to some joint paper publications on the role of tabulated chemistry methods in describing and modelling MILD Combustion conditions in a cyclonic combustor.

Confirmation of the Host Institution of the successful execution of the STSM

See attached letter

Other Comments

I sincerely appreciate the COST office for giving me this valuable opportunity to visit TU/e in Eindhoven, the Netherland. My thanks also go to my colleagues of the Combustion group at IRC-CNR in Naples, Dr Mara de Joannon and Dr. Raffaele Ragucci and the entire team for their support.