SHORT TERM SCIENTIFIC MISSION (STSM) – SCIENTIFIC REPORT

The STSM applicant submits this report for approval to the STSM coordinator

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Grantee name: Giuseppe Ceriello
Home institution: University of Naples Federico II
Host institution: Eindhoven University of Technology (TU/e)

Title: CFD simulation with Flamelet Generated Manifold (FGM) of a cyclonic burner with high level of internal recirculation

PURPOSE OF THE STSM

The main purpose of this activity lies in the advanced numerical simulation of a cyclonic burner operating under MILD [1, 2] conditions, built by the IRC-CNR Research Group of Naples.

The two research groups of Eindhoven and Naples are carrying out a collaboration work to model such a system during last years to the aim of assessing a tabulated chemistry approach (FGM) to MILD combustion systems. The implementation of FGM method [3, 4], in fact, seems to be a promising tool for MILD systems. FGM is based on the tabulation of the chemistry of the system solving simplified 0D or 1D configurations called Flamelet and defining a few controlling variables for which to solve the CFD equations. This model allows the use of detailed kinetic mechanisms which is crucial for a MILD combustion system.

Simulations were already carried out for few cases and compared to the experimental data obtained in Naples. The runs were performed using the software Chem1D to solve the Flamelets whereas the CFD was solved in Fluent using the RANS equations and a presumed beta PDF approach to include the turbulence/chemistry interaction effects. Since the promising results, the model needs to be improved to better fit the different operating conditions and to reproduce the internal burned gas recirculation with heat loss through the environment.

Therefore, the first part of the STSM will involve the numerical setup of the model to enhance the control on the system from a computational point of view (manifold generation, boundary conditions, etc.). Afterwards, a new Flamelet configuration will be solved to include a new table dimension in order to better represent the cyclonic reactive flow with the inclusion of enthalpy as adding controlling variable.

Finally, several test conditions investigated during experimental campaigns performed in Naples, will be simulated by means User Defined Functions and compared to the measured data.

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DESCRIPTION OF WORK CARRIED OUT DURING THE STSM

The work done during the STSM consists mainly in the optimization of the tabulated chemistry model FGM for a MILD cyclonic reactor. Such an optimization was carried out by creating a 3D laminar and non-adiabatic database by means tabulating chemistry from a stationary premixed flamelet in order to include the very low enthalpy levels needed by the system.

Experimental Data and Test Case

Experimental tests conducted in Naples on a laboratory-scale cyclonic flow reactor were available. Figure 1 shows a sketch of the section (a) and the front view (b) of the non-premixed configuration of the laboratory-scale burner used to investigate the MILD/flameless combustion process [5, 6]. It is a small-scale prismatic chamber with a square section (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 preheating levels and injected at around 18 m/s whereas the fuel stream (pure CH_4) is settled at an environmental temperature (T_0=300 K) and around 16 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 0.0015 m. The feeding configuration is shown in Figure 1a. The gas exit is located on the top of the chamber.

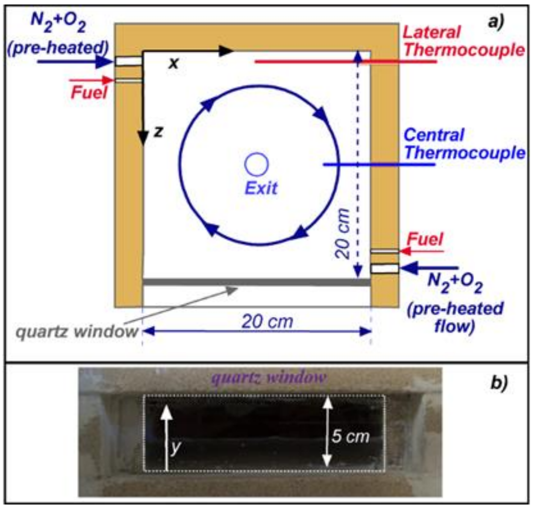


Fig. 1 Sketch of the midplane section (a) and front view (b) of the cyclonic configuration.

The combustor is built using a heat-insulating material, the expanded vermiculite, and it is located within an electrically heated ceramic oven. The main oxidizer flow passes through heat exchangers located within the electrical ceramic fiber heaters to raise the temperature to the desired values, while the fuel is injected at environmental temperature.

The cyclonic burner is equipped with a set of thermocouples (type N) and an optical access (a quartz window) as shown in Figure 1. Two movable thermocouples are located at the mid-plane of 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 centreline of the combustion chamber (0.1 m from the wall) as depicted in Figure 1a. The thermocouples can be moved across the reactor. The exhausts were monitored at the exit of the combustion chamber while the emissions were analysed by means of a GC analyser.

The experimental conditions under attention during the STSM are summarized in Table 1. For all measurements, the global inlet content of N_2 (diluent) is fixed at air conditions. The pressure of the system is atmospheric. During the experimental campaign, the autoignition of the fresh oxidizer charge was reached by increasing the inlet temperature of the oxidizer (by means of external preheating systems) from the environmental temperature to the desired value T_{in}.

CASE	**T_0 (K)**	**T_{in} (K)**	**Φ**	**Y_{O2} / Y_{N2}**	**Vfuel (m/s)**	**Vox (m/s)**	**T walls (K)**
STEC	300	1000	1	0.21/0.79	15.83	17.78	1310
LEAN	300	1000	0.7	0.21/0.79	15.83	17.78	1280
RICH	300	1000	1.3	0.21/0.79	15.83	17.78	1290

Tab. 1 List of the conditions investigated in this study.

By means fixed thermocouples placed at fixed positions on the walls, a mean wall temperature was evaluated and reported in the last column of Table 1.

FGM model

FGM is a chemistry reduction method, which is based on two assumptions: an 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 called Flamelet and tabulating the related quantities as functions of a few controlling variables (CVs). During a CFD simulation, only the transport equations for CV are solved and the required variables are looked-up from the so-called FGM look-up 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 order to compute the Flamelet, the specialized solver Chem1D [7] was used in this work. During previous simulative works about the cyclonic burner, the attention was paid to the Igniting Mixing Layer (IML) approach [8]. In this configuration, fuel and oxidizer are initially placed side-by-side and then mix by molecular diffusion and react in time. However, this configuration does not allow the inclusion of the enthalpy as additional CV in an effective way. In fact, the high heat exchanged by the system with the environment implies that low enthalpy level must be included in the FGM table. In order to do that a stationary premixed flamelet was considered to tabulate the three CVs required: a progress variable (PV) defined as a combination of the mass fractions of H_2O, CO_2 and HO_2; a mixture fraction (Z) computed using Bilger’s formula; and the total enthalpy (H).

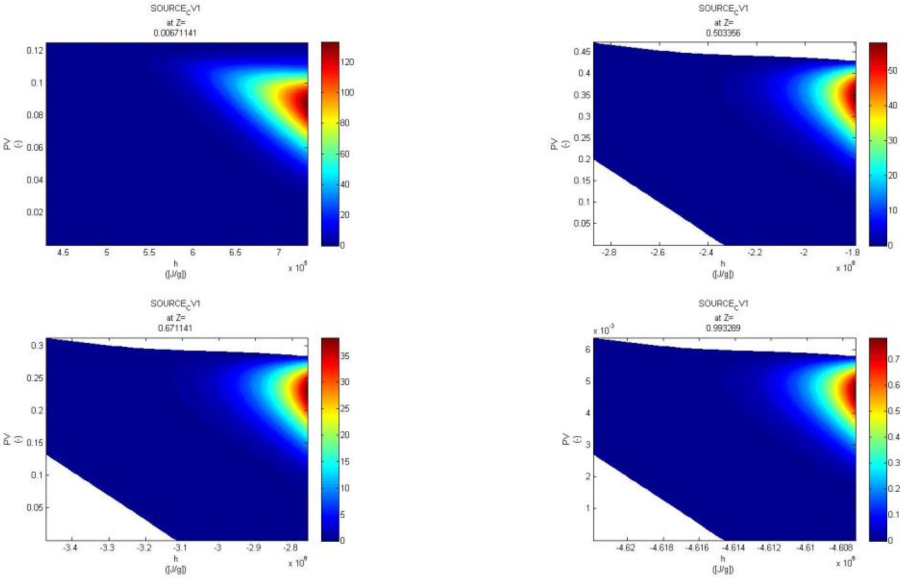


Fig. 2 PV source term manifold as a function of PV and H for four different Z.

The chemistry data obtained by the tabulation procedure is rearranged through a coordinate transform. The tabulated data is then directly retrievable as a function of CVs. An overview of the resulting manifold can be seen in Figure 2, where the PV source term is represented as a function of progress variable and total enthalpy for different Z values.

This dataset is stored in memory and associated to the CFD code. During a simulation, the CVs transport equations are solved in addition to Favre-averaged mass and momentum equations:

$$\frac{\partial \bar{\rho}\tilde{u}_j\tilde{Z}}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\bar{\rho}D + \frac{\mu}{Sc}\right)\frac{\partial \tilde{Z}}{\partial x_j}\right],$$

$$\frac{\partial \bar{\rho}\tilde{u}_j\widetilde{PV}}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\bar{\rho}D + \frac{\mu}{Sc}\right)\frac{\partial \widetilde{PV}}{\partial x_j}\right] + \overline{\omega_Y},$$

$$\frac{\partial \bar{\rho}\tilde{u}_j\tilde{H}}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\bar{\rho}D + \frac{\mu}{Pr}\right)\frac{\partial \tilde{H}}{\partial x_j}\right].$$

Where $\bar{\rho}$ the mean density, $\tilde{u}_j$ is the mean velocity vector, D is the molecular diffusion coefficient, μ is the viscosity, Sc is the Schmidt number, Pr is the Prantl number, $\overline{\omega_Y}$ is the mean chemical source term of the progress variable. The gradient transport assumption [9] coupled with unity Lewis numbers for all variables have been used to model the turbulent diffusion terms.

The FGM considers turbulence-chemistry interaction by describing variables in a stochastic way through a Probability Density Function (PDF). So, the laminar manifold is rearranged in a turbulent database by using an assumed shape PDF-averaging approach [10]. The inclusion of the variances was not performed here since the only laminar table was tested to value the reliability of the premixed configuration for the cyclonic burner. The beta-PDF approach was, however, used testing the database with the FGM option of ANSYS Fluent 18.1.

Numerical methods

The conditions in Table 1 were numerically investigated. The Premixed Flamelets at different equivalence ratios and temperatures were computed on Chem1D. The CFD simulations were performed with the commercial code ANSYS Fluent 18.1 using both the FGM option built in the commercial solver and by using a User Define Function. By means ICEM CFD 18.1 the grid was constructed considering a complete 3D geometry of the combustion chamber. An unstructured computational mesh composed of about 400k hexahedral elements, clustered near the inlets, was used (Figure 3) with all Boundary Conditions (BC) selected. 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 grid provides high resolution in the mixing and reaction regions and close to the inlets and save computational effort elsewhere. Favre-averaged Navier–Stokes equations were solved using Re-Normalization Group (RNG) k-ε turbulence model with swirl dominated flow corrections to account for the high swirl in the combustor and Enhancement Wall Treatment as near-wall modelling method. The mixing field of such combustor was already characterized in a previous work of the same group [48]. It was showed that the high-speed oxidizer jet induces a strong swirl within the reactor and that the fuel jet is strongly bent by EGR, assuring an efficient mixing between flows. The path-line plot confirmed the presence of a strong recirculation of gases inside the combustor, ensuring high residence times. Moreover, large toroidal recirculation zone with a high level of turbulence is established inside the combustor and the high gas recirculation rates promote the attainment of the high temperature and low oxygen concentration conditions required for the stable autoignition of the MILD mixture.

The global kinetic mechanism GRI30 was adopted.

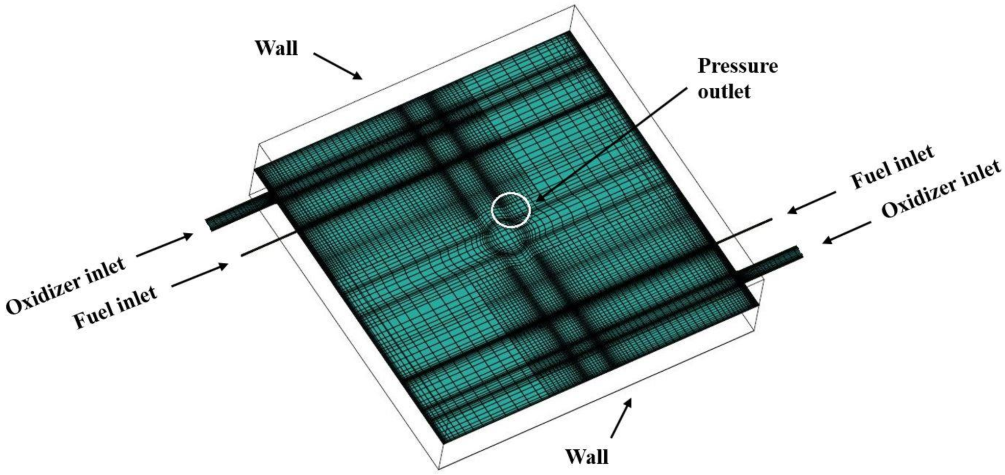


Fig. 3 Three-dimensional view of the geometry, boundary conditions and details of the grid.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

The first preliminary results were obtained by comparing the numerical results with the premixed table to those with IML (non-premixed) using the FGM option of ANSYS FLUENT 18.1. Afterwards the 3D laminar premixed database was tested by using UDF and compared to experimental data.

Comparison premixed/non-premixed tables using Fluent 18.1 FGM

In Figure 4 is shown the comparison between measured data and simulated temperature profiles for two different types of flamelets (IML and PREMIXED) for case STEC (Table 1).

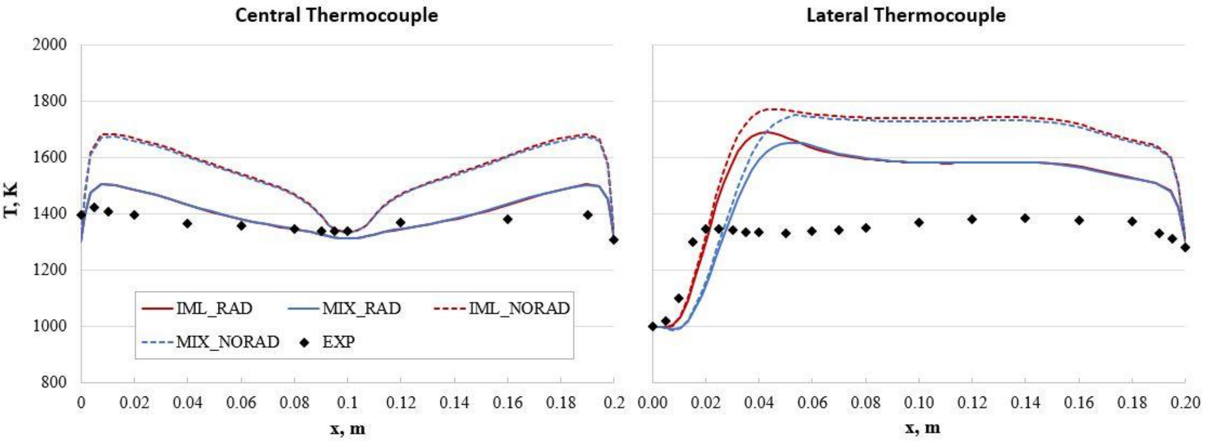
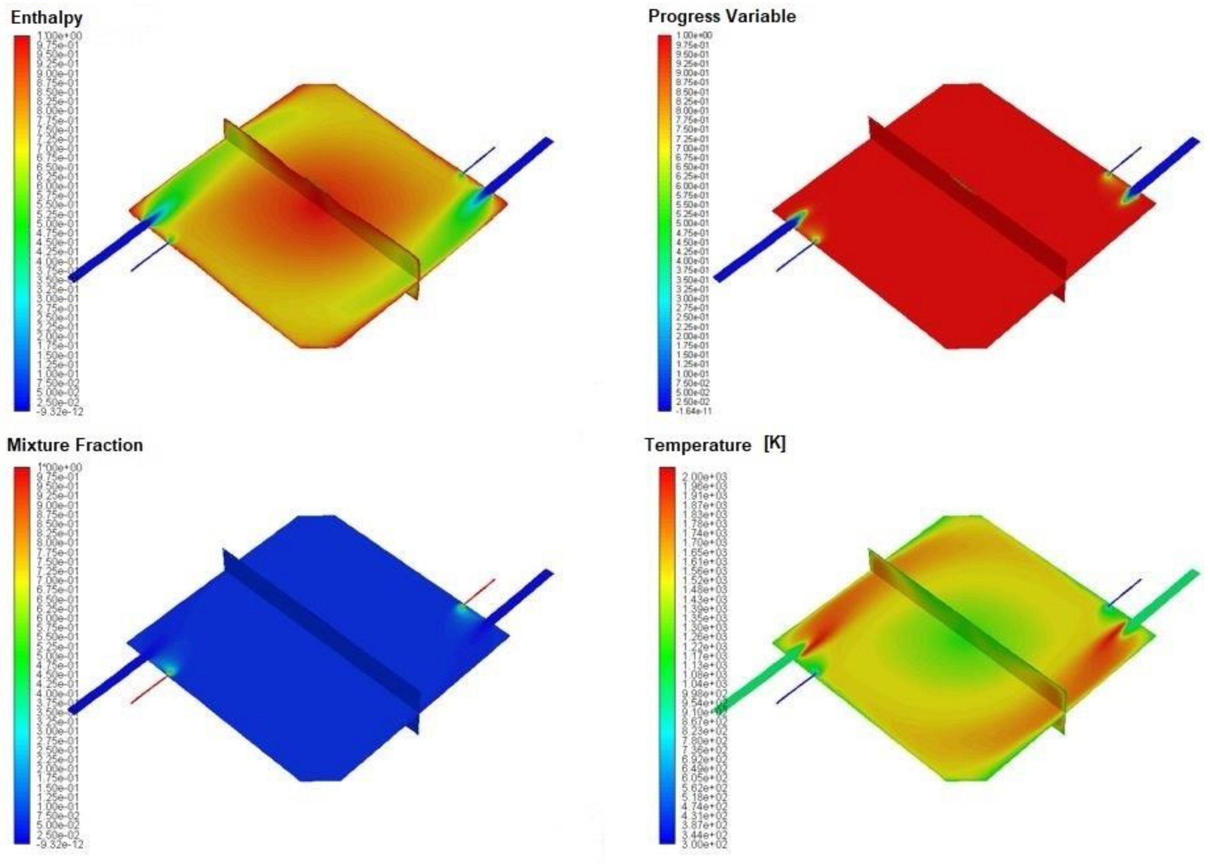


Fig. 4 Comparison between measured data and simulated temperature profiles for two different types of flamelets (IML and PREMIXED) for case STEC.

The simulations in Figure 4 were performed on Fluent by importing the 2D (PV, Z) laminar table and using the FGM option for including variances and enthalpy. Moreover, a DO model was used for radiation in addition to WSGG. It can be noted that the results for the two different flamelet configurations are basically the same except for the zone very near to inlet, where the premixed flamelet delays the ignition and decreases the temperature peak. That means that the CFD simulations of the non-premixed cyclonic configuration are slightly affected by the use of a premixed tabulated flamelet for the tabulation of the chemistry. This proves that the choice of the premixed configuration was valid.

Simulations with 3D laminar table by means UDF

The non-adiabatic and laminar 3D manifold (PV, Z and H as controlling variables) was tested on ANSYS Fluent 18.1 by User Defined Function. In Figure 5 the temperature and CVs contours are reported.



Enthalpy

Progress Variable

Mixture Fraction

Temperature [K]

Fig. 5 Contours at mid planar and vertical planes of the three CVs and temperature for case STEC.

Finally, Figure 6 shows the comparison between the simulated temperature profiles inside the chamber with the 3D laminar table using UDF and both the measured data and the results obtained by Fluent’s FGM.

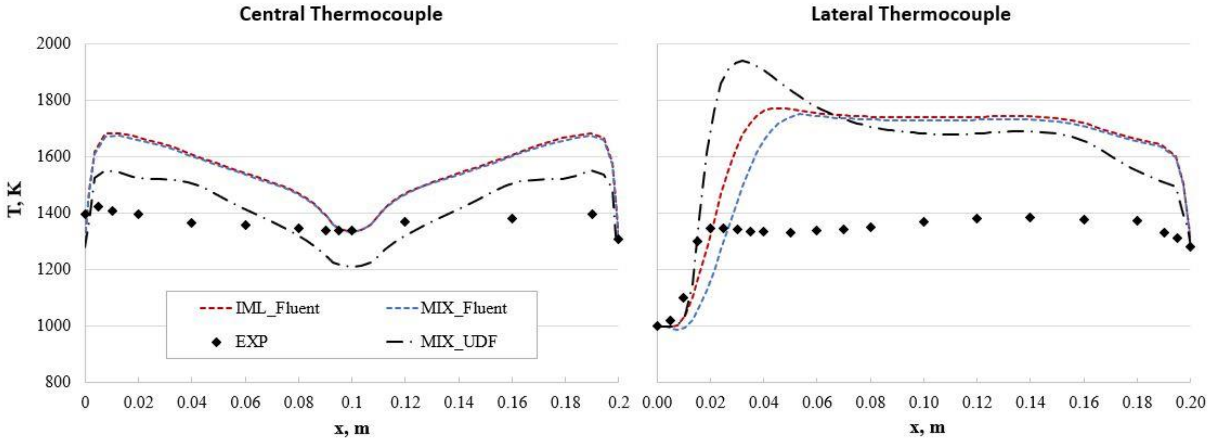


Fig. 6 Comparison between the simulated temperature profiles and measured data and the simulations by Fluent's FGM for the two different Flamelet configuration for case STEC.

The results seem to be promising if we consider that the CV's variances were not included, and the radiative transfer was neglected.

FUTURE COLLABORATION WITH THE HOST INSTITUTION

The scientific collaboration between the IRC-CNR Research Group of Naples and the Multiphase & Reactive Flows Department of the TU/e will be still carried out in the course of the next months in order to improve the preliminary results found during this STSM.

In particular, the effect of the inclusion of the variances (and so the turbulence) will be evaluated. The focus will be also pointed on the optimization of FGM model for the cyclonic MILD burner in an Open FOAM environment.

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