ASSESSMENT OF THE PERFORMANCE OF SEVERAL TURBULENCE AND COMBUSTION MODELS IN THE NUMERICAL SIMULATION OF MILD COMBUSTION IN A LABORATORY COMBUSTOR

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Abstract. In this paper, mild combustion in a laboratorial combustion chamber is numerically simulated. A comparison of different turbulence and combustion models, and different chemical reaction mechanisms is reported, being the results validated using experimental data obtained in a small-scale combustor fired with methane. Turbulence was modeled using four different models: the standard, the realizable and the RNG k- ε models, as well as the Revnolds stress model. Combustion was simulated using also four different models, namely the laminar flamelet model for diffusion flames, two different partially premixed flamelet models and the eddy dissipation concept. One of the partially premixed models combines the laminar flamelet model for diffusion flames with a premixed flame model based on the solution of a transport equation for a non-reacting scalar variable G that represents the normal distance to the flame front. The other one is a simple combination of a premixed model based on the solution of a transport equation for a progress variable, and the non-premixed flamelet model for diffusion flames. Three different chemical reaction mechanisms are compared: a global one-step reaction, the DRM-19 and the GRI-2.11 mechanisms for methane combustion. The calculations show that the different turbulence models employed do not yield significant differences for the studied conditions, as far as the mean temperature, oxygen and carbon dioxide molar fraction profiles are concerned. The three models based on the flamelet concept predict a too steep rise in temperature and CO_2 mole fraction along the combustor axis in comparison with the experimental data, even though they yield satisfactory predictions elsewhere. In contrast, the eddy dissipation concept along with a detailed reaction mechanism yields rather good predictions, particularly if the most detailed reaction mechanism is employed. The global one-step reaction does not satisfactorily reproduce the experimental data.

1 INTRODUCTION

Flameless oxidation is a combustion regime where the reactants are highly diluted with hot combustion products, causing the reactions to occur in a distributed reaction zone with a reduced temperature maximum, smooth temperature gradients and low oxygen partial pressure. In this regime, distinct flame fronts, as they occur in typical lean premixed or diffusion flames, are replaced by a volume type flame mode. As a consequence, the temperature distribution is nearly uniform and NO_x emissions are very low. The reduction of the aero-acoustic fluctuations and extended stability limits are additional benefits of this combustion regime. This technology has received various names, such as high temperature air combustion (HiTAC) [1], flameless oxidation (FLOX[®]) [2], moderate or intense low oxygen dilution (MILD) combustion [3] and colorless distributed combustion (CDC) [4], with a number of studies revealing the success of this technology as a NO_x control technique.

Coelho and Peters [5] carried out numerical simulations of a flameless oxidation burner based on the solution of the Favre-averaged Navier-Stokes equations. The turbulence-chemistry interaction was accounted for by means of the non-premixed flamelet – probability density function (PDF) approach. The NO_x emission was calculated by the Eulerian particle flamelet model in a post-processing state. They argued that the steady flamelet library was unable to correctly describe the formation of NO, because this is a chemically slow process, which is sensitive to transient effects, while the unsteady flamelet model was able to predict the correct order of magnitude of NO_x emissions. Mancini et al. [6, 7] presented numerical simulations of flameless combustion in a semi-industrial furnace. They used the standard k- ε turbulence model together with three combustion sub-models: the eddy-breakup model with a two-step reaction scheme, the eddy-dissipation concept model (EDC) with chemical equilibrium, and the mixture fraction/PDF model with equilibrium tables. The three combustion models provide predictions of similar quality. The numerical models have correctly reproduced the uniformity of the temperature and oxygen fields. However, the combustion models could not describe the chemistry and temperature field in the fuel jet region. Parente et al. [8] investigated the influence of the combustion model and kinetic mechanism on the MILD combustion of hydrogen enriched fuels in an industrial burner. They claim that the eddy dissipation model is unable to describe the features of MILD combustion, while the EDC performs well if a detailed chemical mechanism is used. However, a detailed assessment of the models is prevented by the lack of detailed measurements inside the combustor. Kumar et al. [9] presented numerical simulations of a flameless combustion test facility. They used the EDC model with a skeletal chemical reaction mechanism, and included an extinction model based on the Damköhler (Da) number. The flame is assumed to be quenched when the fluid time scale is smaller than the chemical time scale (Da < I). The chemical time scale is derived as a function of temperature, oxidizer mass fraction, fuel dilution, velocity of the jet and fuel type, while the fluid time scale is obtained from the k- ε turbulence model. The predictions of this model are satisfactory. Finally, Duwig et al. [10] studied flameless oxidation in a model gas turbine combustor using large eddy simulation and a combustion model based on a progress variable. The instantaneous source term is obtained from tabulated data, which was calculated from detailed chemical kinetics and based on an unsteady perfectly stirred reactor approach. The mean source term is computed using a presumed filtered density function. The model along with the experimental data allowed the determination of the flameless operation regime in terms of fuel/air ratio.

Despite of the studies above, the present knowledge on the theoretical foundations of the MILD combustion phenomena is still limited. In particular, there is a lack of detailed experimental data available to provide increased insight into the underlying physics, and the success in accurate simulations of this combustion regime has been limited so far. This article presents a numerical study of a laboratory combustor fired with methane under MILD combustion conditions. A comparison of different turbulence and combustion models, and different chemical reaction mechanisms is reported, being the results validated using experimental data.

2 EXPERIMENTAL COMBUSTOR

The combustion chamber is a cylinder with a diameter of 150 mm and a length of 300 mm as shown in Figure 1. The burner is placed at the top end of the combustion chamber and the exhaust of the burned gases is made by the bottom end through a convergent nozzle with a length of 50 mm and an angle of 35°. Along the length of the combustion chamber there are 5 ports, each with a diameter of 20 mm, which allow for the introduction of probes inside the combustion chamber. The chamber is equipped with electrical elements that allow preheating the combustor walls up to ≈ 900 °C. Two thermocouples installed in the combustion chamber are used to monitor the wall temperatures and to evaluate the temperature gradients along the combustor. The burner consists of a central gas gun and a combustion air supply in a conventional double concentric configuration. The combustion air is preheated by an electrical system that allows inlet temperatures up to \approx 750 °C. The sampling of the gases for the measurement of local mean O₂, CO, CO₂, unburned hydrocarbons (HC) and NO_x molar fractions was achieved using a stainless steel water-cooled probe. The analytical instrumentation included a magnetic pressure analyzer for O_2 measurements, a non dispersive infrared gas analyzer for CO₂ and CO measurements, a flame ionization detector for HC measurements and a chemiluminescent analyzer for NO_x measurements. Local mean temperature measurements were obtained using uncoated 76 µm diameter fine wire platinum/platinum:13% rhodium thermocouples. The analog outputs of the analyzers and of the thermocouple were transmitted via A/D boards to a computer where the signals were processed and the mean values computed. Flue-gas data were obtained using the same procedures. More details about the experimental installation are given in [11].

Experimental conditions	1	2
Power kW	10.0	15.6
λ	2.0	1.6
Air temperature injection (°C)	500	700
Air mass flow rate (g/s)	6.9	8.4
Air inlet velocity (m/s)	102.1	158.4
Re_{Dh} air inlet	14.0×10^{3}	14.9×10^{3}
Methane temperature injection (°C)	20	20
Methane inlet mass flow rate (g/s)	0.2	0.31
Methane inlet velocity (m/s)	24.4	38.1
Wall temperature (°C)	900	980

Table 1 presents the combustor operating conditions used to perform the measurements and the computational simulations.

Table 1: Experimental conditions.



Figure 1: Experimental combustor.

3 MATEMATICAL MODELS

The mathematical model is based on the numerical solution of the Favre-averaged governing equations for mass, momentum and energy and on transport equations related to the turbulence and combustion models. Most previous works were based on the standard k- ε model or on some variant, such as the realizable or RNG versions, to model turbulence. We have tested all these variants, as well as the Reynolds stress model.

The thermal radiation was taken into account using the discrete ordinates method (DOM) and the radiative properties of the participating medium were modelled by the weighted-sum-of-grey gases model (WSGGM) in which the spatial variation of the total emissivity is computed as a function of the H_2O and CO_2 local mass fractions and temperature.

Two kinetic mechanisms were considered to describe the methane oxidation, the DRM-19 [12] and the GRI-2.11 [13]. The DRM-19 mechanism is a subset of the GRI-1.2 full mechanism, developed to obtain the smallest set of reactions needed to closely reproduce the main combustion characteristics predicted by the full mechanism. It consists of 19 species, plus Ar and N₂. The GRI-2.11 mechanism consists of 277 reaction steps involving 47 species.

3.1 Turbulence/chemistry interaction models

Turbulence/chemistry interactions have been modelled using five different models: the Eddy Dissipation Model/Finite Rate (EDM/FR), the Eddy Dissipation Concept (EDC), the steady laminar flamelet model for diffusion flames and two partially premixed models also based on the flamelet concept.

EDM/FR

The EDM/FR is a simple and computationally cheap model for describing the turbulence/chemistry interactions. According to this model, a mixing rate, $\overline{\omega}_{i,EDM}$, and

an Arrhenius rate, $\overline{\omega}_{i,FR}$, both based on the mean properties, are evaluated and the smallest one is chosen as the mean reaction rate for the reacting species, i.e., $\overline{\omega}_i = \min(\overline{\omega}_{i,FR}, \overline{\omega}_{i,EDM})$.

For a global mechanism with a single irreversible reaction, the source term of species *i* obtained by the Arrhenius rate may be written as:

$$\overline{\omega}_{i,FR} = M_i \left(v_i'' - v_i' \right) \left(K \prod_{j=1}^{N_j} \left(C_j \right)^{n_j' + n_j''} \right) \tag{1}$$

where M_i represents the molar mass of species *i*, v'_i and v''_i are the stoichiometric coefficients of reactant and product species *i*, respectively, C_j the molar concentration of species *j* in the mixture and *K* the Arrhenius reaction constant.

The source term of species *i* obtained by the EDM approach is calculated from [14]:

$$\overline{\omega}_{i,EDM} = \min\left[\nu_i' M_i A \overline{\rho} \frac{\varepsilon}{k} \min\left(\frac{\tilde{Y}_r}{\nu_r' M_r}\right), \nu_i' M_i A B \overline{\rho} \frac{\varepsilon}{k} \left(\frac{\sum_{j=1}^{N_p} \tilde{Y}_j}{\sum_{j=1}^{N_p} \nu_j' M_j}\right)\right]$$
(2)

where, $\overline{\rho}$ is the mean density of the mixture, \tilde{Y}_r represents the mass fraction of the reactant species in defect on the mixture, i.e., oxygen for rich conditions and fuel in the case of lean combustion, and N_p represents the number of products of the reaction. A and B are model constants set equal to 4.0 and 0.5, respectively.

EDC Model

The EDC model proposed by Magnussen (see [15]) is an extension of the EDM that allows the use of detailed chemistry. According to the EDC model, combustion occurs in the regions of the flow where the dissipation of turbulent kinetic energy takes place. Such regions are denoted as fine structures and they can be described as perfectly stirred reactors. The mass fraction of the fine structures, γ_{λ} , and the mean residence time of the fluid within the fine structures, τ^* , are evaluated from an energy cascade model, which describes the energy dissipation process as a function of the characteristic scales

$$\tau^* = 0.41 \left(\frac{\nu}{\varepsilon}\right)^{1/2} \tag{3}$$

$$\gamma_{\lambda} = 2.13 \left(\frac{\nu \varepsilon}{k^2}\right)^{1/4} \tag{4}$$

where v is the kinematic viscosity, and ε and k are the dissipation of turbulent kinetic energy and turbulent kinetic energy, respectively. The mean source term in the conservation equation for the *i*th species is modelled as:

$$\overline{\omega}_{i} = -\frac{\overline{\rho}\gamma_{\lambda}^{2}}{\tau^{*}} \frac{\left(\tilde{Y}_{i} - Y_{i}^{*}\right)}{\left(1 - \gamma_{\lambda}^{3}\right)}$$
(5)

where Y_i^* is the mass fraction of the *i*th species inside the fine structures and \tilde{Y}_i is the Favre mean mass fraction obtained from:

$$\tilde{Y}_i = \gamma_\lambda^3 Y_i^* + \left(1 - \gamma_\lambda^3\right) Y_i^0 \tag{6}$$

where Y_i^0 represents the species *i* mass fraction in the fluid surrounding the fine structures.

Flamelet Model

The laminar flamelet model relies on the assumption that combustion chemistry is fast and occurs in thin layers, the so-called flamelets, embedded within the turbulent flow. The width of these layers is assumed to be smaller than the Kolmogorov length scale which implies a scale separation between combustion and turbulence in the inertial range [16]. The flamelet equations may be derived by applying a coordinate transformation with the mixture fraction Z as a new independent coordinate to the governing equations for the temperature and the species mass fraction. This leads, after neglecting lower order terms, to the unsteady flamelet equations [17]:

$$\rho \frac{\partial T}{\partial t} - \rho \frac{\chi}{2} \frac{\partial^2 T}{\partial Z^2} - \rho \frac{\chi}{2c_p} \frac{\partial T}{\partial Z} \frac{\partial c_p}{\partial Z} -\sum_i \left(\rho \frac{\chi}{2} \frac{c_{pi}}{c_p} \frac{\partial Y_i}{\partial Z} \frac{\partial T}{\partial Z} \right) + \frac{1}{c_p} \sum_i \dot{w}_i h_i + \frac{q_R}{c_p} = 0$$

$$\rho \frac{\partial Y_i}{\partial t} - \rho \frac{\chi}{2} \frac{\partial^2 Y_i}{\partial Z^2} - \dot{w}_i = 0$$
(8)

where ρ is the density, *T* the temperature, χ the scalar dissipation rate, c_p the specific heat capacity, *t* the time, \dot{w} the reaction rate, *h* the enthalpy and q_R the radiative source per unit volume. In the derivation of these equations it was assumed that the Lewis number for all the species is unity. The density is then obtained using the ideal gas equation of state.

The steady flamelet library was generated by means of the solution of the flamelet equations for several values of the scalar dissipation rate ranging from a low value close to equilibrium to a high value close to extinction.

The scalar dissipation rate in the flamelet equations can be expressed for onedimensional flows as a function of the mixture fraction. This function may be taken from a counter-flow geometry [17] as:

$$\chi(Z) = \frac{a}{\pi} \exp\left\{-2\left[\operatorname{erfc}^{-1}(2Z)\right]^2\right\}$$
(9)

where *a* is the velocity gradient in the oxidizer stream. This relation may also be written as:

$$\chi(Z) = \chi_{st} \frac{f(Z)}{f(Z_{st})}$$
(10)

where f(Z) is the exponential term that appears on the right of the equation (9) and the subscript *st* denotes stoichiometric conditions. The turbulent effects were accounted for by integrating the laminar values over the mixture fraction space using an assumed beta probability density function (PDF), P(Z):

$$\tilde{\chi} = \frac{\tilde{\chi}_{st} \int_{0}^{1} f(Z) \tilde{P}(Z) dZ}{f(Z_{st})}$$
(11)

where $\tilde{\chi}$ is the sink term of the transport equation for the variance of the mixture fraction, which is modelled by:

$$\tilde{\chi} = C_x \frac{\varepsilon}{k} \widetilde{Z''^2}$$
(12)

In this equation C_x is set equal to 2.0.

If the steady flamelet equations are solved, then the inclusion of the radiative source term in the flamelet equation yields unrealistic results, as shown in [18]. Therefore, the radiative source term was not included in the flamelet equations, and the mean temperature calculated from equation (7) was ignored. The temperature was computed from the local mean enthalpy as:

$$\tilde{h} = \sum_{i=1}^{n} h_i(\tilde{T}) \tilde{Y}_i$$
(13)

The enthalpy equation solved in the CFD code includes a radiative source term computed from the radiation model. The local mean values of the species mass fractions are obtained from integration of the solution of equation (8) for the scalar dissipation rate at stoichiometric conditions:

$$\tilde{Y}_{i}(\vec{x}) = \int_{0}^{1} Y_{i}(Z, \tilde{\chi}_{st}) P(Z) dZ$$
(14)

The mean mass fractions of the species are stored in a library as a function of the mean mixture fraction, its variance and the scalar dissipation rate.

Partially premixed model A

The model A is a partially premixed turbulent combustion model based on the solution of a transport equation for a non-reacting scalar variable G, which represents the normal distance to the flame front. This *G*-equation may be derived from the local kinematics relation between the propagation velocity of a flame front in the unburnt mixture and the local flow velocity [19]. The flame position is defined by $G(\vec{x}, t)_{flame} = G_o$, where G_o is an arbitrary constant fixed at the flame front. This surface divides the flow field in two regions such that $G > G_o$ is the region of the burnt gas and $G < G_o$ is the region of the unburnt gas. The solution of the *G* equation allows the clear identification of the flame front position in the flow field. The time-averaged form of this equation may be written as [16]:

$$\frac{\partial \overline{\rho} \tilde{G}}{\partial t} + \nabla \cdot \left(\overline{\rho} \tilde{v} \tilde{G} \right) = \overline{\rho} S_f \left| \nabla \tilde{G} \right| - \overline{\rho} D_t \kappa \left| \nabla \tilde{G} \right|$$
(15)

where κ is the curvature of the mean flame front and D_t is the turbulent diffusivity, which can be determined from the relation $D_t = 0.78\nu'' l_t$, where ν'' is the root mean square velocity and l_t is the turbulent length scale computed from:

$$l_t = C_D \frac{k^{3/2}}{\varepsilon} \tag{16}$$

 C_D is a constant with the value of 0.37.

The turbulent burning velocity S_T is usually defined with respect to the unburnt mixture. A mass balance at the flame front provides the relation between the turbulent flame velocity, S_T , and the local velocity of the flame front, S_f

$$S_f = \frac{\overline{\rho}_u S_T}{\overline{\rho}} \tag{17}$$

Here ρ_u is the density of the unburnt mixture immediately upstream of the flame front and ρ is the density of the mixture at the flame front. The turbulent burning velocity was computed using the model proposed by Chen et al. [20]. This model uses PDF to account for the influence of fluctuations of the mixture fraction field, upstream of the flame front, in the turbulent burning velocity:

$$S_{T} = \int_{0}^{1} S_{L}(Z) P(Z) dZ + v'' \int_{0}^{1} \left[-0.195 Da(Z) + \sqrt{\left(0.195 Da(Z)\right)^{2} + 0.78 Da(Z)} \right] P(Z) dZ$$
(18)

where Da(Z) is the turbulent Damköhler number, which can be expressed as:

$$Da(Z) = \frac{S_L^{2}(Z)l_t}{v''D}$$
(19)

where D is the mass diffusivity, which can be evaluated by using the relation $D = S_L l_F$, where S_L is the laminar flame speed and l_F is the flame thickness computed from $l_F = 1.78 l_t$.

In the flow field, the local mean value of the mass fraction of species *i* is calculated from:

$$\widetilde{Y}_{i} = f_{b}\widetilde{Y}_{i,b} + (1 - f_{b})\widetilde{Y}_{i,u}$$
(20)

where f_b is the fraction of burnt material in the control volume under consideration, and $\tilde{Y}_{i,b}$ and $\tilde{Y}_{i,u}$ are the local mean mass fractions of species *i* for a burnt diffusion flamelet and a quenched diffusion flamelet, respectively. The mass fractions of the chemical species are obtained from the flamelet library. The fraction of burnt material in each control volume, f_b , is obtained by assuming that the *G* fluctuations satisfy a Gaussian distribution [20]:

$$f_b = \int_{G=G_0}^{\infty} \frac{1}{\sqrt{2\pi \widetilde{G}''^2}} \exp\left[-\frac{\left(G - \widetilde{G}\right)^2}{2\widetilde{G}''^2}\right] dG$$
(21)

The parameter f_b is equal to zero at control volumes with unburnt material, one for control volumes with burnt material, and ranges from zero to one inside the turbulent flame brush.

The variable G represents a distance, as mentioned earlier. In order to enforce G to remain a distance function during the iterative process, the G field is updated every iteration using the algorithm described in [21].

Partially premixed model B

The partially premixed model B is based on the premixed model presented in [22], and involves the solution of a transport equation for the reaction progress variable. In

this model, the progress of the reaction is the same as the progress of the flame front. The flame front propagation is modelled by solving a transport equation for the scalar quantity \tilde{c} , the Favre averaged reaction progress variable:

$$\frac{\partial \overline{\rho} \tilde{c}}{\partial t} + \nabla \cdot \overline{\rho} \tilde{v} \tilde{c} = \nabla \cdot \left(\frac{\mu_t}{Sc_t} \nabla \tilde{c} \right) + \overline{\rho} S_c$$
(22)

where Sc_t is the turbulent Schmidt number and S_c represents the reaction progress source term. The reaction progress variable is defined as:

$$c = \frac{\sum_{i=1}^{N_p} Y_i}{\sum_{i=1}^{N_p} Y_{i,ad}}$$
(23)

where $Y_{i,ad}$ the mass fraction of species *i* after complete adiabatic combustion. Based on this definition, c = 0 in the unburnt mixture and c = 1 in the burnt mixture. The source term in equation (22) is modelled as:

$$\overline{\rho}S_c = \overline{\rho}_u S_T \left| \nabla c \right| \tag{24}$$

The turbulent flame velocity was computed using a model for wrinkled and thickened flame fronts [22]:

$$S_T = A(v'')^{3/4} S_L^{1/2} \alpha^{-1/4} l_t^{1/4}$$
(25)

where A is a constant of the model and α the thermal diffusivity of the unburnt mixture. The value 0.52 is proposed for A. The model relies on the assumption of equilibrium of small-scale turbulence inside the flamelet, resulting in a turbulent flame velocity that is a function of the large-scale turbulent parameters.

The partially premixed model is a simple combination of the premixed and the nonpremixed models. The premixed reaction-progress variable determines the position of the flame front. Downstream of the flame front (c = 1), the mixture is burnt and the laminar flamelet mixture fraction solution is used. Upstream of the flame front (c = 0), the species mass fraction, temperature and density are calculated from the mixed but unburnt mixture fraction. Within the flame (0 < c < 1), a linear combination of the unburnt and burnt mixture is used. The mean species mass fractions are calculated from:

$$\tilde{Y}_{i} = \tilde{c}\tilde{Y}_{i,b} + (1 - \tilde{c})\tilde{Y}_{i,u}$$
(26)

Under the assumption of thin flames, only unburnt reactants and burnt products exist.

4 RESULTS AND DISCUSION

The calculations were carried out using two 2-dimensional axisymmetric, nonuniform grids. The grids have a higher density in the region near the burner exit and in the vicinity of the centreline. The coarsest grid has 42×130 nodes and the finest one has 83×229 nodes in the radial and axial directions, respectively. The computational domain extends 870 mm beyond the exhaust of the combustion chamber for both grids. No significant differences were observed between the solutions obtained with the two grids, so the results are considered grid independent. The results presented in this work were obtained using the finest grid.

At the inlet boundaries, the radial velocity component at the burner exit was taken as zero, and the axial velocity was calculated from the fuel and air mass flow rates, respectively. The inlet turbulent kinetic energy, \tilde{k}_{in} , was estimated by assuming that the turbulence intensity is either 5% or 10%, No differences were observed in the results for these two distinct conditions. The results presented in this paper refer to the case that assumes 10% intensity of the turbulence at the inlet boundaries. The inlet values of the dissipation rate of the turbulent kinetic energy were determined from $\tilde{\varepsilon}_{in} = 0.169 \tilde{k}_{in}^{1.5}/l$. The mixing length, *l*, was taken as the hydraulic radius of the fuel and air injectors. The wall temperature was set equal to the measured value.

The simulations with the two partially premixed models were performed using an in-house CFD code, while the commercial code Fluent 6.23 was used for the others cases. The commercial software COSILAB was used to compute the laminar flame velocity for different degrees of premixing and temperatures of the unburnt mixture. The computed laminar flame velocity is stored in a library as a function of the mean mixture fraction and the unburnt temperature. The values of temperature and mixture fraction upstream of the flame front were used to interpolate the laminar flame velocity and calculate the turbulent flame velocity.

The convergence criterion demanded that the sum of the residuals of the energy equation decrease below 10^{-6} and the sum of the residuals for all the other variables decrease below 10^{-4} .

4.1 Influence of the turbulence model

Figures 2 and 3 present measured and predicted temperature and species molar fraction radial profiles for condition 1 (see Table 1) obtained using different turbulence models. All the simulations were performed using the EDC with the GRI-2.11 kinetic mechanism. The temperature predictions of the various models are similar and, in general, there are no significant differences between the computational results and the measurements. However, in the near burner region the simulations underestimate the temperature values. At 150, 210 and 270 mm downstream of the burner, in the vicinity of the centreline, the temperatures predicted by the realizable k- ε model are lower than those predicted by the other models and also lower than the experimental values.

The O₂ and CO₂ molar fractions predicted by the standard and the realizable k- ε models are similar and, in general, are in good agreement with the experimental values. Nevertheless, in the centreline at x = 150 mm, the molar fractions of O₂ predicted by the realizable k- ε model are higher than the experimental data and the predictions of the k- ε standard model. Consistently, at this location, the temperatures and CO₂ molar fraction predicted by the realizable k- ε model are lower than the experimental data and the predictions of the standard k- ε model.

The molar fractions of O_2 obtained by the RNG k- ε model and the RSM, in the recirculation zone of the combustor, are lower than those calculated using the other models and experimentally determined. Consistently, the CO₂ molar fraction predictions exhibit the opposite behaviour. This is most evident in the two profiles close to the top of the combustor (x = 30 mm and 90 mm). The O₂ and CO₂ molar fractions predicted further downstream by the various turbulence models are closer to each other and to the experimental data. However, the RNG k- ε model and the RSM overpredicted the CO₂ molar fractions and underpredicted the O₂ molar fractions in the axis of the combustion chamber near the exhaust. In part these results explain the poor predictions obtained by these two models in the recirculation zone on the top of the combustor. In fact, molar fractions of the species are a function not only of the local reaction rate associated with these species, but also a function of the amount of O₂ and CO₂ transported by the flow from regions downstream.

The predicted CO molar fractions exhibit large discrepancies in comparison with the experimental results, regardless of the turbulence model used. Nevertheless, both the measurements and the computational values are lower than one percent, and therefore the impact of the poor predictions of the CO molar fractions on the temperature field is marginal.



Figure 2: Measured and predicted radial temperature and O_2 molar fraction profiles for condition 1 obtained using different turbulence models. (Symbols: measurements; — $k - \varepsilon$ standard; — $k - \varepsilon$ RNG; — $k - \varepsilon$ realizable; — RSM)



Figure 3: Measured and predicted radial CO₂ and CO molar fraction profiles for condition 1 obtained using different turbulence models. (Symbols: measurements; — k- ε standard; — k- ε RNG; — k- ε realizable; — RSM)

4.2 Influence of the kinetic mechanisms

Figures 4 and 5 present the measured and predicted radial profiles of temperature and species molar fractions obtained using the standard k- ε model and the EDC model with the two kinetic mechanisms considered in this study (DRM-19 and GDI-2.11). In general, the computational results do not differ significantly among themselves. However, Figure 4 shows that the detailed reaction mechanism yields better predictions of the temperature in the region far from the burner. At 210 and 270 mm downstream of the burner, the simulation carried out using the DRM-19 mechanism underpredicts the temperature in comparison with the experimental values, especially in the vicinity of the centreline.

The largest discrepancies for the chemical species occur in the prediction of the CO molar fractions. Both kinetic mechanisms strongly overpredict the measured CO mass fraction. The GRI-2.11 kinetic mechanism performs better in the recirculation zone near

the combustion chamber wall, while the results obtained using the DRM-19 kinetic mechanism are in better agreement with the experimental values near the axis of the combustor.

The numerical results for the O_2 and CO_2 molar fractions predicted by the two reaction mechanisms are in close agreement with each other, except the profile located 30 mm downstream of the burner, where the predictions of the O_2 molar fractions obtained using the DRM-19 kinetic mechanism are lower and these of CO_2 are higher than the predictions obtained using the GRI-2.11 kinetic mechanism. At these locations, the predictions of the detailed mechanism are in better agreement with the experimental results.



Figure 4: Measured and predicted radial temperature and O₂ molar fraction profiles for condition 1 obtained using different kinetic mechanisms. (Symbols: measurements; --- DRM-19; --- GRI-2.11)



Figure 5: Measured and predicted radial CO₂ and CO molar fraction profiles for condition 1 obtained using different kinetic mechanisms. (Symbols: measurements; — DRM-19; — GRI-2.11)

4.3 Influence of combustion model

Figures 6 and 7 show the measured and predicted radial profiles of the temperature and species molar fractions (O₂, CO₂ and CO) for condition 1. Obtained using the five combustion models considered in this study. All the simulations were performed using the standard k- ε turbulence model.

In the recirculation zone, the predictions of the temperatures and molar fractions of O_2 and CO_2 are in very good agreement with the experimental data for all models. However, the results obtained using the different combustion models exhibit significant differences in the near burner region. The diffusion flamelet model predicts high temperatures and molar fractions of CO and CO_2 , along with low values of O_2 molar fraction, 30 mm downstream of the burner. These results clearly indicate that the diffusion flamelet model considers an intense chemical activity near the burner, as in the conventional diffusion flames, which is not supported by the measurements.

Further downstream, the three models based on the flamelet approach show similar results. While the diffusion flamelet model predicts an intense combustion process near the burner, the partially premixed models prevent the combustion process to occur so intensely in the region immediately downstream of the burner, where they yield lower predicted temperatures. However, after this initial zone, the diffusion flamelet and the partially premixed models predict too high temperatures and too low species (O₂, CO₂) molar fractions, which is not supported by the experimental data. In the region where the variable G employed in the partially premixed model A is lower than zero, the molar fractions of the species and the temperature change only due to the mixing process between the combustion air, the recirculated products and the fuel. Downstream of this initial region, G becomes greater than zero, and outside the thin layer that represents the turbulent flame thickness, the model A become identical to the flamelet model for diffusion flames. This explains the predicted strong rise of the temperature, and of the molar fraction of CO_2 , and the reduction of the O_2 concentration from x = 30 mm to x = 90 mm. This reasoning is also valid for model B, i.e., downstream of the initial region of the combustor, where variable c has values between zero and one, the model is identical to the flamelet model for diffusion flames.

These results clearly show the inability of the flamelet and partially premixed models to predict the MILD combustion process in the region near the burner. The flamelet approach assumes fast chemistry with Da >> 1 and, as suggested in [23], MILD combustion is a process where the chemical time scale and the turbulence time scale are of the same order of magnitude.

The predictions of the EDM/FR and EDC are similar in the near burner region. Downstream, the results obtained using EDM/FR move progressively towards the predictions of the three models that use the flamelet approach. In the region near the burner, characterized by an extremely intense mixing process with high dissipation, the EDM/FR assumes that the combustion process is limited by chemical reactions. The discrepancy between the results obtained by the EDM/FR and the EDC shows the limitations of the global kinetic mechanism in the prediction of the combustion process near the axis of the combustor at 150 and 210 mm downstream of the burner. In this region of the combustor, the dissipation rate becomes lower. The EDM/FR assumes fast chemistry and the combustion is controlled by the turbulent mixing process. Therefore the results of the EDM/FR become closer to those based on the flamelet approach.

In general, the EDC is the model that performs best. The EDC predictions of temperature and molar fractions of O_2 and CO_2 are in good agreement with the experimental results. However, in the near burner region, the model underestimates the temperatures and the molar fraction of O_2 and slightly overestimates the molar fraction of CO_2 . The quality of the results in this zone may be affected by the limitations of the turbulence model to predict accurately the development of the jet and the mixing process between the combustion air and flue gas recirculation in the near burner region.

The CO molar fractions predicted by the EDC model near the exit of the combustion chamber and in the recirculation zone significantly exceed the experimental values, but remain smaller than 1%.



Figure 6: Measured and predicted radial temperature and O₂ molar fraction profiles for condition 1 obtained using five different combustion models.
(Symbols: measurements; — EDC; — EDM/FR; — partially premixed model A; — partially premixed model B; — turbulent diffusion flamelet model)



Figure 7: Measured and predicted radial CO₂ and CO molar fraction profiles for condition 1 obtained using five different combustion models.
(Symbols: measurements; — EDC; — EDM/FR; — partially premixed model A; — partially premixed model B; — turbulent diffusion flamelet model)

Figure 8 shows the measured and predicted radial profiles of the temperature and the O_2 molar fractions, obtained using the EDC, with the GRI-2.11 mechanism, for conditions 1 and 2. These simulations were performed using the standard *k*- ε turbulence model. The results show that the predictions for condition 2 are worse than for condition 1. The simulations for condition 2 predict an evolution of the combustion process slower than that experimentally observed. In the recirculation zone, the predictions are good for both conditions. It is not clear why the performance of EDC the model is different for these two conditions.



Figure 8: Measured and predicted radial temperatures and O₂ mole fraction profiles obtained using the EDC/GRI-2.11 model, for conditions 1 and 2.
(Symbols: measurements; — simulation condition 1; — simulation condition 2)

5 CONCLUSIONS

The main conclusions of this study are as follows:

- The standard k- ε model provides the best results. However, the quality of the simulations is not significantly affected by the turbulence models.
- The simulations made using the EDC model show that the quality of the simulations is broadly independent of the chemical kinetics mechanism used.
- The results clearly show the inability of the models based on the flamelet concept to predict the MILD combustion process. The partially premixed models only prevent the combustion process to occur so intensely in the region immediately downstream of the burner.

• Among the combustion models evaluated in the present work, the EDC is the best one in the prediction of MILD combustion. Nevertheless, the predictions of CO molar fraction and the predictions obtained for condition 2 exhibit shortcomings, and therefore the results are still not entirely satisfactory. According to this, there is a strong need to develop new combustion models that take into consideration the specific nature of the MILD combustion phenomenon, namely the fact that the fuel mixes and reacts with a mixture of air and combustion products, rather than with pure air, as in conventional diffusion flames.

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