Numerical Simulation of a Small-Scale Mild Combustor

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Abstract. This work reports numerical simulations of a small-scale cylindrical combustor operating in the mild combustion regime. Preheated air is supplied by a central nozzle, while the fuel (methane) is injected through 16 holes placed equidistantly in a circumference concentric with the air nozzle. The calculations were carried out using the commercial code Ansys-Fluent. Turbulence was modelled using the realizable $k$-$\varepsilon$ model. Two different combustion models were employed, namely the eddy dissipation concept and the joint composition pdf transport model. In both cases, a chemical mechanism comprising 13 transported species and 73 chemical reactions was used, as well as a global single-step reaction. A thorough comparison of the predictions obtained using the pdf transport model and the eddy dissipation concept with detailed experimental data is presented. Both models are able to accurately predict the temperature and the $O_2$ and $CO_2$ molar fractions over most of the combustor, but the temperature field is overestimated in the vicinity of the burner. Discrepancies are found in the prediction of the $CO$ molar fraction, particularly when the eddy dissipation concept is used.

1. Introduction

The mild combustion regime was identified about twenty years ago, during the course of experimental work independently carried out in Germany, Japan, and The Netherlands [1-3]. Since then, mild combustion has been employed in several industrial sectors due to its advantages in comparison with conventional combustion processes. It is characterized by a volumetric instead of a thin reaction zone and, consequently, a more uniform temperature field with lower turbulent temperature fluctuations than in conventional combustion processes. In some conditions, the flame becomes invisible. The NO and CO emissions are low, as well as the noise. Mild combustion is achieved by means of a strong recirculation of combustion products, and significant dilution of the oxidant with the combustion products occurs prior to reaction with the fuel. The temperature of the walls of the combustion chamber is generally high, and the oxidant is often pre-heated.

Despite the success demonstrated so far by mild combustion, more experimental research, particularly detailed data inside the combustion chamber, is needed to improve current understanding of the underlying physical and chemical processes, and to allow validation of mathematical models, in order to promote further transfer of this technology to the industry. In this context, several research groups have been involved in the numerical simulation of combustion chambers operating in the mild combustion regime, even though the validation is often limited due to the lack of detailed experimental
data. These studies comprise a wide range of geometries and modelling approaches.

Most simulations of mild combustion have been based on the solution of the Reynolds-Averaged Navier-Stokes equations using the standard, the realizable or the RNG versions of the $k$-$\varepsilon$ model, or the Reynolds stress model. Comparisons of the performance of these turbulence models are reported in [4-7]. There is no evidence in the literature of superior performance of the realizable or RNG versions of the $k$-$\varepsilon$ model or of the RSM over the standard $k$-$\varepsilon$ model in the modelling of the mild combustion regime. The interaction among different physical phenomena is likely to be the main reason for the satisfactory predictions of the standard $k$-$\varepsilon$ model in comparison with other potentially more accurate turbulence models. Large eddy simulation has also been used to model mild combustion, as reported in [8-9].

Several different combustion models have been used in the simulations published in the literature. The conserved scalar/prescribed pdf formulation has been used along with a chemical equilibrium assumption [4, 10-12] or with the laminar flamelet model [7, 13-15]. It has been argued that these models are inadequate, since they rely on the assumption of fast chemistry, while the dilution of the reactants with combustion products in the mild combustion regime slows down the chemistry in such a way that typical Damköhler numbers are low. Simple models, such as the eddy break-up, the eddy dissipation and the eddy dissipation/finite rate models were used with limited success in [4-5, 10], [4, 10-12] and [7, 12, 16], respectively. Mancini et al. [5] used a model based on a network of perfectly stirred reactors. Duwig et al. [8] developed a model that describes the combustion process by unsteady perfectly stirred reactors. The initial temperature and mass fraction of the species are defined as a linear function of the burnt and unburnt states, and the dilution coefficient is tabulated as a function of progress variables for the temperature and fuel mass fraction. Several authors have reported a good performance of the eddy dissipation concept [18] in the modelling of mild combustion [6-7, 19-24]. The conditional moment closure was used in [25], and the transport pdf method was employed in [26].

In the present work, a laboratory scale mild combustor is numerically simulated using two different combustion models, namely the EDC and the composition pdf transport model. Apart from the application to a free jet in a hot co-flow reported in [26], we are not aware of previous modelling of a combustion chamber operating in the mild combustion regime using the composition pdf transport model. The predictions are compared with detailed experimental data.

2. Mathematical Modelling

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. Turbulence was modelled using the realizable $k$-$\varepsilon$ model [27], which involves the solution of transport equations for the turbulent kinetic energy and its dissipation rate. Two different combustion models were used, namely the EDC [18] and the joint composition pdf transport model [28].

The EDC is an improved version of the eddy dissipation model [29], which is able to use detailed finite-rate chemical kinetics in the simulation of turbulent reactive flows. Transport equations for the species are solved during the CFD calculations, so that the computational requirements are higher than those of models based on the conserved scalar formulation with a prescribed pdf shape, such as the laminar flamelet model, in which the chemistry is decoupled from the CFD calculations and tabulated. However, models based on this formulation rely on the fast chemistry assumption. The EDC is not restricted to fast chemistry flows, and is able to simulate both high and low Damköhler number flows.

The EDC relies on the Kolmogorov cascade of energy dissipation on all length scales in turbulent flows from the largest eddies to the smallest ones, in which turbulent kinetic energy is converted into heat through viscous friction. The model assumes that chemical reactions, as well as molecular mixing associated with turbulence dissipation, occur within the fine structures of the flow, defined as a small fraction of the total fluid volume where the reactants are homogenously mixed, similarly to a well stirred reactor. In this model, the mass fraction occupied by the fine structure regions is expressed as a function of the turbulent kinetic energy, its dissipation rate and the kinematic viscosity. The reactions
are assumed to occur in the fine structures over a residence time scale, and the mean reaction rate in the conservation equation for the species is inversely proportional to that time scale.

The composition joint pdf (C-PDF) transport model is an alternative method for modelling chemically reacting turbulent flows, which provides an effective solution to the closure problem that arises from averaging the highly nonlinear chemical source terms. This model calculates the composition joint probability density function of the temperature and mass fractions of chemical species. Their mean values are evaluated from the composition joint pdf, which satisfies a transport equation [28]. In this equation, the highly non-linear reaction term is completely closed and requires no modelling. This is the main advantage of this model. However, the terms describing convection by turbulence and the molecular mixing/diffusion need to be modelled. The first one was modelled using the gradient diffusion assumption, while the second one was modelled using the Euclidean Minimum Spanning Tree [30]. This mixing model takes into account the physical position of the stochastic particles that are adjacent to each other, which makes this model the most accurate mixing model available in the CFD code used in this work. The joint pdf transport equation was solved using the Monte Carlo method. Notional particles with mass move randomly through the physical space, due to particle convection, and through the composition space, due to molecular mixing and chemical reactions, in fractional time steps, allowing the position, the temperature and the mass of the particles to be found after every time step.

A skeletal chemical mechanism for the combustion of methane comprising 13 transported species and 73 chemical reactions was used [31]. Calculations performed using a global methane-air reaction mechanism [32] are also reported. The in-situ adaptive tabulation (ISAT) method [33] was used to reduce the computational cost of the chemical source term integration for both the EDC and the C-PDF methods.

Thermal radiation was taken into account using the discrete ordinates method and the radiative properties of the participating medium were modelled using the weighted-sum-of-grey gases model, in which the spatial variation of the total emissivity is computed as a function of the \( \text{H}_2\text{O} \) and \( \text{CO}_2 \) local mass fractions and temperature.

3. Experimental Set-up and Techniques
The experimental details can be found in [34] and a short description is given here. Figure 1 shows a schematic of the combustor used in this study. The combustion chamber is a quartz-glass cylinder with an inner diameter of 100 mm and a length of 340 mm. The burner is placed at the top end of the combustion chamber and the exhaust of the burned gases is through the bottom end. The burner consists of a central orifice of 10 mm inner diameter, through which the combustion air is supplied, surrounded by 16 small orifices of 2 mm inner diameter each, positioned on a circle with a radius of 15 mm, for the fuel (methane) supply. The combustion air is preheated by an electrical heating system that allows air inlet temperatures up to 700 ºC, which are monitored using a type K thermocouple installed at the entrance of the burner.

Local mean temperature measurements were obtained using 76 µm diameter fine wire platinum/platinum:13% rhodium (type R) thermocouples. The uncertainty due to radiation heat transfer was estimated to be less than 5% by considering the heat transfer by convection and radiation between the thermocouple bead and the surroundings.

The sampling of the gases for the measurement of local mean \( \text{O}_2 \), \( \text{CO}_2 \) and \( \text{CO} \) molar fractions was achieved using a stainless steel water-cooled probe. The analytical instrumentation included a magnetic pressure analyzer for \( \text{O}_2 \) measurements and a non dispersive infrared gas analyzer for \( \text{CO}_2 \) and \( \text{CO} \) measurements. The major sources of uncertainty in the concentration measurements inside the combustor were associated with the quenching of chemical reactions and aerodynamic disturbances of the flow. Quenching of the chemical reactions was rapidly achieved upon the samples being drawn into the central tube of the probe due to the high water cooling rate in its surrounding annulus – our best estimate indicated quenching rates of about \( 10^7 \) to \( 10^8 \) K/sec. On average, the repeatability of the gas species concentration data was within 10%. Both the temperature and the gas species probes were
inserted into the quartz-glass combustion chamber through holes made on the bottom end of the combustor.

The operating conditions simulated here correspond to an excess air coefficient, defined as the actual air-fuel ratio to the stoichiometric air-fuel ratio of 1.3, an inlet air temperature of 700 ºC, and a thermal input of 10 kW. The inlet velocities of air and fuel are 157.5 m/s and 6.1 m/s, respectively.

![Figure 1. Schematic of the combustor.](image)

**Figure 1.** Schematic of the combustor.

**Figure 2.** Computational grid.

### 4. Computational Details

The computational domain corresponds to a section of 1/16 (22.5º) of the combustion chamber. The mesh has approximately 137,000 control volumes, and is shown in Fig. 2. The fuel and air ducts are included in the computational domain, in order to allow the flow to develop and to reduce the uncertainty in the definition of the boundary conditions for the turbulent kinetic energy and dissipation rate at the entrance to the combustor. The grid is structured, except in the transition between zones of different refinement, with rectangular control volumes over a large part of the computational domain, and non-uniform, being more refined close to the inlets, in the vicinity of the burner region and mixing zones.

Uniform axial velocity profiles of air and fuel were prescribed at the inlet section of the admission ducts. The turbulent kinetic energy and the dissipation rate were prescribed using the method suggested in [35]. Standard wall functions were used for the velocity boundary conditions at the walls of the combustor. The wall temperature was set to 1400 K, based on experimental measurements. Outlet pressure with zero gauge pressure was set for the boundary condition at the exhaust.

All the governing equations were solved using a second order upwind discretization scheme, and the SIMPLEC algorithm. The calculations performed using the C-PDF model were carried out using 10 particles per control volume. The convergence criterion demanded that the sum of the residuals of the discretized equations over the domain dropped below 10^{-3}, except for the energy conservation equation, where a tolerance of 10^{-6} was used. In addition, it was requested that the values of the temperature, the O_2 and the CO_2 mass fractions at several monitoring points of the computational domain, become approximately constant during the course of the iterative solution process.
5. Results and Discussion
The predicted velocity field in a plane defined by the axis of the combustor and the axis of the fuel duct is shown in Fig. 3. These results were obtained using the C-PDF along with the skeletal reaction mechanism. The large momentum of the inlet air jet originates an internal recirculation zone that extends up to about 80% of the length of the combustor. The recirculated hot combustion products transport momentum and energy back to the top of the combustor, where they mix with the incoming fuel. The mass flow rate of fuel is much lower than the mass flow rate of recirculated combustion products, so that the fuel jet hardly penetrates through the combustion products. The fuel entrains the flow of recirculated combustion products, and mixes with them before ignition, which takes place in a diluted environment, as required in mild combustion.

Figure 4 shows predicted and measured profiles of mean temperature and mean molar fractions of O$_2$, CO$_2$ and CO (dry basis) along the axis of the combustor. The axial profiles of mean temperature determined using the C-PDF display small oscillations, which are due to the relatively small number of stochastic particles used in the simulations. These oscillations disappear with the increase of the

![Figure 3. Predicted velocity field.](image)

![Figure 4. Predicted and measured axial profiles of mean temperature, O$_2$, CO$_2$ and CO molar fractions on a dry basis.](image)
Figure 5. Predicted and measured radial profiles of mean temperature, $O_2$, $CO_2$ and $CO$ molar fractions on a dry basis.
number of particles, but then the computational time is very high, particularly if the skeletal mechanism is employed. Overall, the predictions are in relatively good agreement with measurements, particularly those obtained using the skeletal mechanism. The global reaction mechanism yields worst predictions, as expected. Nevertheless, none of the models describes accurately the combustion process downstream of the burner, namely in the region $x = 50$ to $x = 150$ mm, where $x$ denotes the axial coordinate. In all cases, the increase of the measured temperature along the centreline is faster than the predicted one. The predicted axial evolution of the molar fraction of major species is in fairly good agreement with the measurements when the skeletal mechanism is employed, but both combustion models underestimate the CO$_2$ molar fraction downstream of the burner. The EDC yields a significant overprediction of the peak of CO molar fraction, even though the location of this peak in very good agreement with the experimental data. The axial profile of CO obtained using the C-PDF model is much closer to the experimental one.

Radial profiles of mean temperature and molar fractions of O$_2$, CO$_2$ and CO are displayed in Fig. 5. These profiles lie in a plane defined by the axis of the combustor and the axis of the fuel duct. The mean temperature profiles at $x = 11$, 45 and 79 mm predicted using the EDC model exhibit a peak at $r \sim 10$ mm, overpredicting the measured values. The maximum values of the measured temperature are closer to the centreline of the combustor than the computed ones. The temperature profiles are consistent with an overprediction of CO$_2$ and CO molar fractions, and an underprediction of O$_2$ molar fraction. The mean temperature calculated using the C-PDF model along with the skeletal mechanism is closer to the experimental data in that region, as well as the maximum values of the CO molar fraction, but there are only marginal differences in the CO$_2$ and O$_2$ molar fraction in comparison with the EDC/skeletal mechanism results. The CO spreads significantly over the radial direction, while the predicted profiles are narrower and closer to the centreline. The EDC model consistently overestimates the CO molar fraction, while the C-PDF model globally performs better as far as the prediction of CO is concerned, but not satisfactorily.

The temperature of the combustion products in the recirculation zone is consistently overpredicted by all models. This may be due to the influence of the prescribed temperature and/or emissivity of the walls on the predictions. This influence is likely to be larger than in conventional combustion processes. In fact, the temperature of the wall is quite high in the present mild combustor, and therefore the radiation emitted by the wall is significant compared with the emission from the medium, and may influence the temperature of the gases. This issue deserves further investigation. In general, the results obtained using the global mechanism show greater discrepancies with the measurements, as also observed above for the axial profiles.

6. Conclusion
A computational study of a laboratory combustion chamber operating in the mild combustion regime is reported. Turbulence is modelled using the realizable $k$-$\varepsilon$ model, and combustion is modelled using the EDC or the composition pdf transport model. A skeletal mechanism for methane is used, as well as a global single-step reaction. Overall, both combustion models along with the skeletal mechanism yield predictions in reasonable good agreement with the experimental data. However, discrepancies have been observed downstream of the burner, where the temperature tends to be overestimated and the predicted profiles exhibit maximum values at a larger radial coordinate. The predictions of CO are not satisfactory, particularly for the EDC model. The results computed using the skeletal mechanism are closer to the experimental data than those calculated using a single-step global reaction.

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