Numerical Simulation of Premixed Combustion Flows:
a Comparative Study

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Abstract

In this work four different commercial and research CFD codes have been compared for the simulation of two combustion test cases. The aim was to get an overview of the capabilities of these different tools to simulate combustion flows in premixed regimes. Codes tested were Fluent, CFX, StarCD and Tanit. Three combustion models have been applied, namely the Eddy Break Up, the Eddy Dissipation Model and the Turbulent Flame Closure, the turbulence model used being the standard k-epsilon. Numerical results have been found to fairly fit experiments and helped to show some drawbacks of combustion models. In its theoretically correct range of applicability the TFC model has been found to give the better agreement with experiments.

Introduction

Premixed combustion is becoming more and more relevant in the industrial combustion technologies being one of the approaches that can make possible to achieve very low pollutants emissions. Design and optimisation of modern burners does rely more and more on the use of CFD tools. Commercial and research CFD codes have reached a good level of sophistication and today they include a number of physical models which are available to describe different combustion regimes offering the user a variety of approaches to best fit his needs.
The most important requirement for a model which has to be used in industrial application is its capability of correctly describing chemistry. This is the challenge of turbulent combustion [1]. For example, at given turbulence conditions, the Eddy Dissipation Model gives a dependence on chemistry which is quasi-laminar overestimating in this way the dependence on temperature [2]. On the other hand, the Turbulent Flame Closure is a model that is able to give more correct dependence on chemistry, as it has been shown in [3].
Assumed that correct dependency on chemistry is very important in evaluating the real capability of a combustion model to represent industrial combustion processes, the model itself has to be able to reproduce experimental data in a very accurate way. But even this is not enough. In fact, the same importance has the ability of a model to give correct answer for trends, that is to give prediction on what the behaviour of the system will be in different conditions. In this work the

three most diffused commercial CFD packages have been tested, namely: CFX, Fluent, and StarCD. Besides the research solver Tanit [4] has been also considered.

Being turbulent premixed combustion the physical phenomenon of interest, only some of the models which can be applied to this regime have been taken into account. In particular only the Eddy Break Up (EBU) [5], the Eddy Dissipation Model (EDM) [6], and the Turbulent Flame Closure (TFC) [7] have been investigated.

The chosen test cases are two turbulent premixed combustion flows in experimental combustors of simple geometry for which a wide spectrum of experimental data exists [8, 9].

Combustion models.

The Eddy Break Model [5] is based on two main ideas: the mixture can be thought as made of completely reacted and completely unreacted gas; the flame region draws inside the fresh mixture, like a jet-flow entrains the fluid from its surroundings. Then the trapped mixture burns with a rate which depends on the local level of turbulence. This dependence is expressed in the source term for the consumption/production of chemical species by the presence of the macroscopic turbulent time scale.

The Eddy Dissipation Model [6] relates the combustion reaction velocity with the dissipation rate of turbulent eddies. The source term for chemical reactions is then expressed accounting for the level of turbulent kinetic energy, the rate of dissipation of turbulent kinetic energy and the mean reactants concentration.

The Turbulent Speed Closure [7] is based on the concept of a turbulent premixed flame brush formed by thickened wrinkled flamelets. The source term for chemical reactions depends on the turbulent flame speed which is defined as a function of the properties of both the laminar flame and the local turbulence.

Test Cases Description

The combustor hereinafter indicated as "Moreau" [8] is shown in Fig. 1. The combustor is fed with a methane-air mixture with equivalence ratio = 0.87. The flame is ignited and stabilised using a burned gas flow entering the lower part of the combustion chamber. The inlet conditions used for the CFD calculation are those summarised in Table 1.

The second test case carried out is the combustor named ENSMA [9]. As shown in Fig. 4 a flame holder is used in order to stabilise the flame. The propane-air mixture composition and fluid dynamics properties of the flow at inlet section are shown in Table 2 and Fig. 5.

Moreau Combustor Results

Figure 2 shows the average x-velocity profiles in a section of the combustor located at 650 mm from inlets. The exam of Fig. 2 indicates a wide scattering of the results obtained using the EBU-class models with exception of the StarCD one which is near to what can be achieved by using TFC model. Accordingly, the same trend has been found for the methane concentration, as shown in Fig. 3.

Moreau Combustor Discussion

Simulations based on the EBU model do fail in reproducing the velocity because they give a too low burning rate. In fact, the low combustion intensity determines an insufficient acceleration of products (see Fig. 2). A tuning of this combustion model in order to better fit the experimental data led to unphysical results i.e., produced a flame lip attached to the upper wall. This effect, due to the turbulent time scale included in the expression of the EBU source term [5], leads to excessively large source term values near solid walls. This problem has been overcome by StarCD which allows the user to make use of a turbulent time scale averaged on the whole flow-field. The results obtained using the TFC model show light differences depending upon the solver which has been used. However, all of them are in good agreement with experiments. Furthermore the TFC is also capable to fairly reproduce the flame brush width as shown in Fig. 3 which presents methane concentration profiles. In contrast from the same figure is quite evident that the EBU based calculations cannot follow properly the slope of the experimental data, leading to an unrealistic too thin flame brush.

ENSMA Combustor Results

Profiles of average x-velocity at 10 mm behind the flame holder are plotted in Fig. 6. In this case the recirculation zone behind the obstacle is fairly reproduced by the EBU based calculations, not by the TFC based ones. The analysis of Fig. 7 shows a general overestimation of peak temperature, while the profile's slope is fairly reproduced. Moving further downstream, both peak temperature and profile's shape are not well captured by all the models, as shown in Fig. 8.

ENSMA Combustor Discussion

The present test case has been found particularly difficult to solve. Any attempt of using EBU model did fail in achieving physically consistent results. Simulations performed using EDM and TFC models raised a series of questions which led the authors to make a deeper analysis of this test case. From fluid-dynamics point of view, calculations have shown a too high level of turbulent kinetic energy behind the flame holder. This behaviour could have at least two possible reasons: a) the turbulence intensity level imposed at inlet was too high; b) the used standard model may fail in describing properly the complex recirculating flow. Both these hypothesis have been investigated by the authors. At first only the inlet turbulence intensity has been reduced in order to better fit the measured turbulence level behind the flame holder. The obtained turbulent kinetic energy profile is the one labelled "TFC-LowK" in Fig. 9, 10 and 11. The exam of Fig. 10, in particular, shows the achieved improvement in the velocity profile due only to the modified turbulence level imposed at inlet. Then both RNG and RSM turbulence models have been used to try and get further amelioration in the solution quality. The same figures show the obtained results. Summarising: the lowering of value at inlet has improved the quality of results even for the simple standard model, but the best solution can be obtained only by using more sophisticated turbulence models.
A second issue is whether the combustion model applied is really effective for simulating this flame. An analysis had then to be performed in order to classify the ENSMA flame. Figure 12 shows the Borghi diagram [10] for premixed combustion regimes, together with the representative points of the two test cases carried out in this work. The exam of this figure shows that the ENSMA flame falls in the thick flames regime, whereas the Moreau flame lays in the premixed

thickened wrinkled flamelets regime. Being the TFC model soundly based on the thickened wrinkled flamelets physical background [7], the model itself is to be expected to fail in reproducing the ENSMA flame. Nevertheless it has been found able to give some qualitative insights even in this case.

Conclusions

In this work the capabilities of four different premixed combustion model of giving qualitatively and quantitatively results on two test cases have been examined. On the only basis of what presented here some conclusions can be achieved. In particular:

In the Moreau test case, which fully fit the wrinkled thickened flamelets regime, TFC model gives the best results, almost independently from which solver has been used. This is not surprising because TFC model is based on this flamelets combustion mechanism [7]. The fact that this regime is quite common in industrial gas turbine could suggest that TFC model is actually able to give the best results also in real applications.

The definition of the flame regime is a preliminary and necessary condition for the choice of the right combustion model to use for each specific problem. As doesn't exist an universal turbulence model, so doesn't exist an universal combustion model either.

The authors do not recommend the ENSMA test case to validate turbulent combustion models which have to be used to simulate industrial combustors. In fact the analysis of the Borghi's diagram [10] (Fig. 12) shows that the combustion regime is almost laminar, being very close to the Reynolds number unit line. This is a situation which is quite impossible to achieve in real applications. Nevertheless this test case remains useful to study fundamental phenomena like, for example, counter gradient transport [9].

The best results for a specific test case depend on the connection of the right turbulence and combustion models. It has been shown how a better resolution of the turbulent flow field leads to a significantly improvement in the quality of the achieved results, even if in situations which are limits for the combustion model.

Acknowledgement
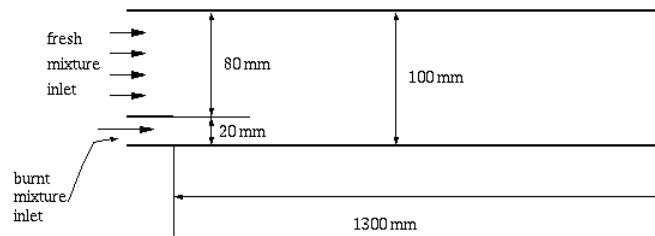
Fig. 1: Moreau combustor geometry.

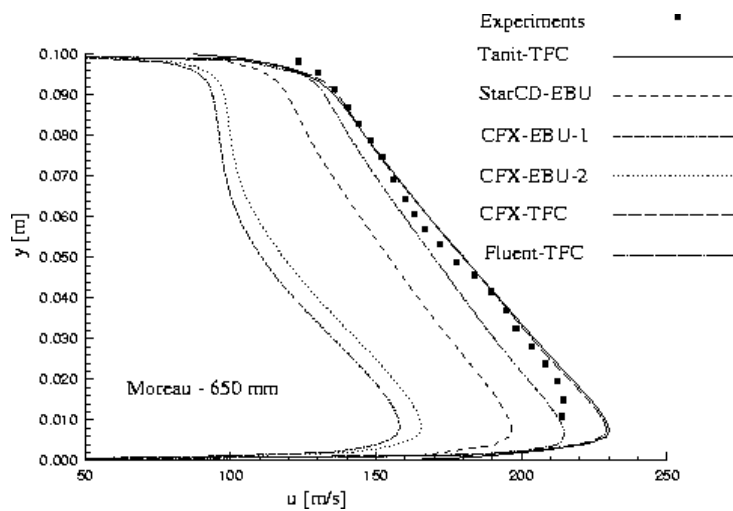|	Burnt gas inlet	Unburned gas inlet
U [m/s]	108	65
V [m/s]	0	0
turb. intensity	21%	12%
turb. lenght scale [m]	0.0014	0.0056
Equivalence ratio	0.87	0.87
Temperature [K]	2000.0 (2200.0)	600.0

Tab. 1: Inlet conditions for Moreau combustor simulation.

Fig.2: Average x-velocity profiles at 650 [mm] from inlet section.
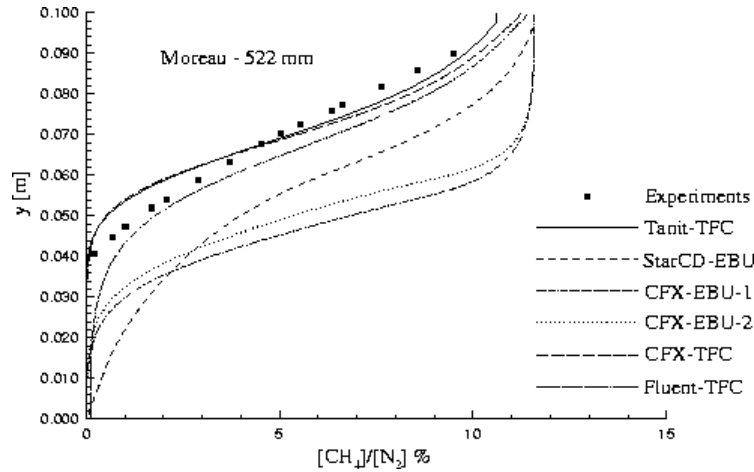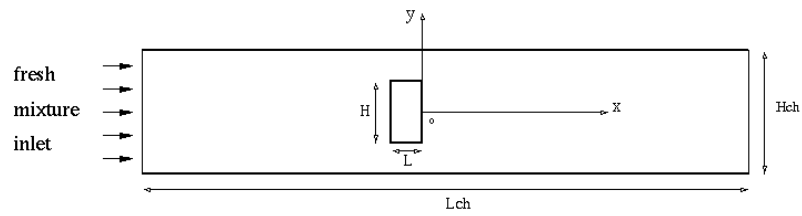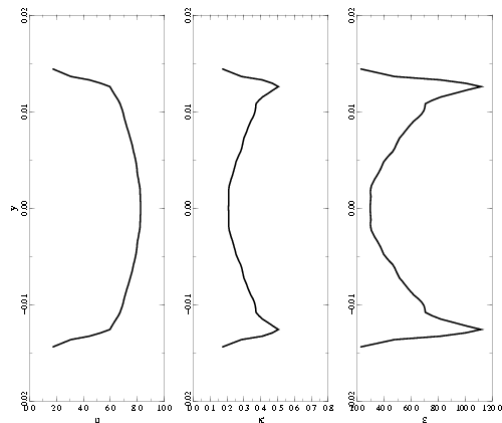
Fig. 3: Average methane concentration at 522 [mm] from inlet section.

Fig. 4: ENSMA combustor geometry.

	Unburned gas
Y(C3H8)	0.04515
Equiv. Ratio	0.65
T [K]	293.0

Tab. 2: Inlet conditions for ENSMA combustor simulation.

Fig. 5:   Inlet profiles for x-velocity, y-velocity and turbulent kinetic energy.
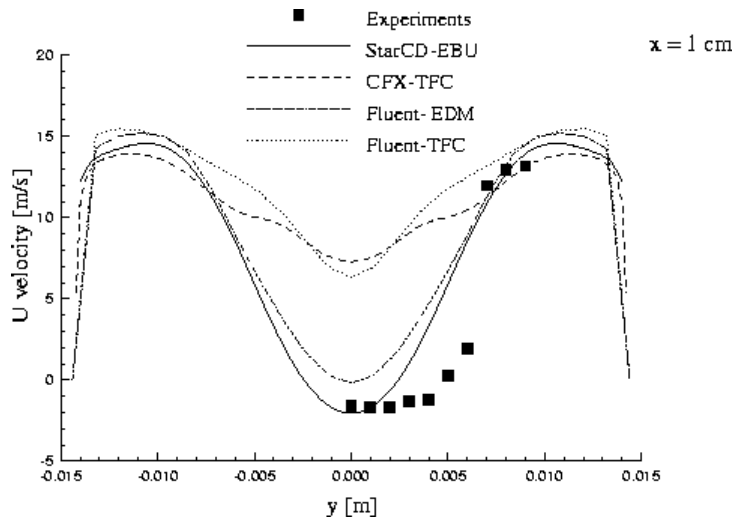
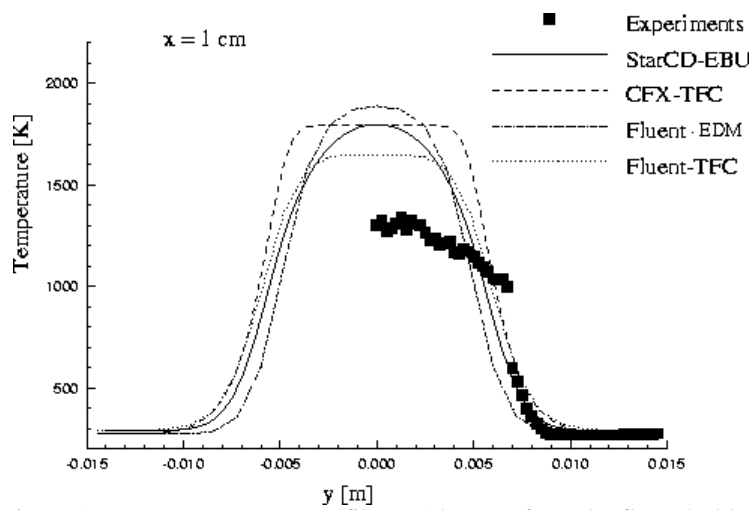Fig. 6: Average x-velocity at 10 [mm] from the flame holder.

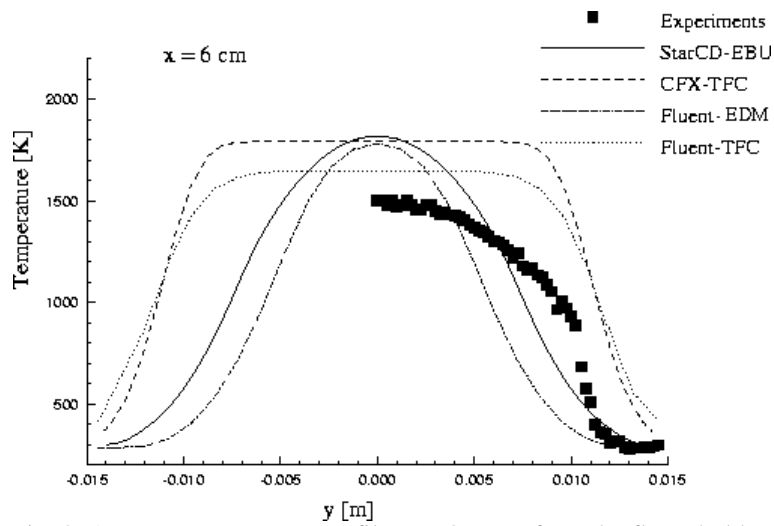Fig. 7: Average temperature profiles at 10 [mm] from the flame holder.

Fig. 8: Average temperature profiles at 60 [mm] from the flame holder.
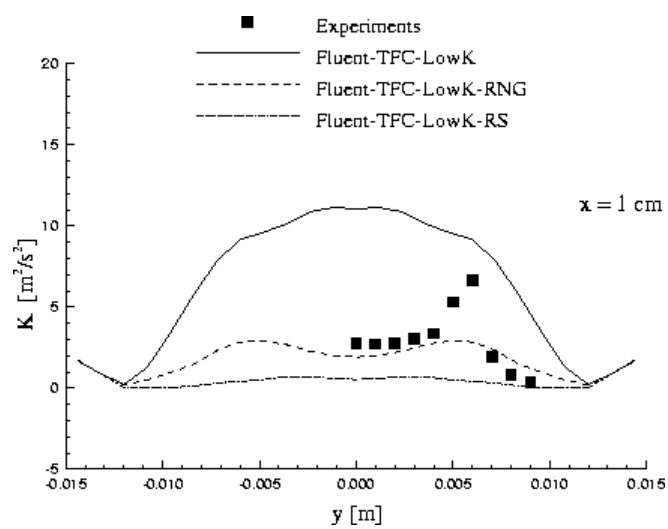

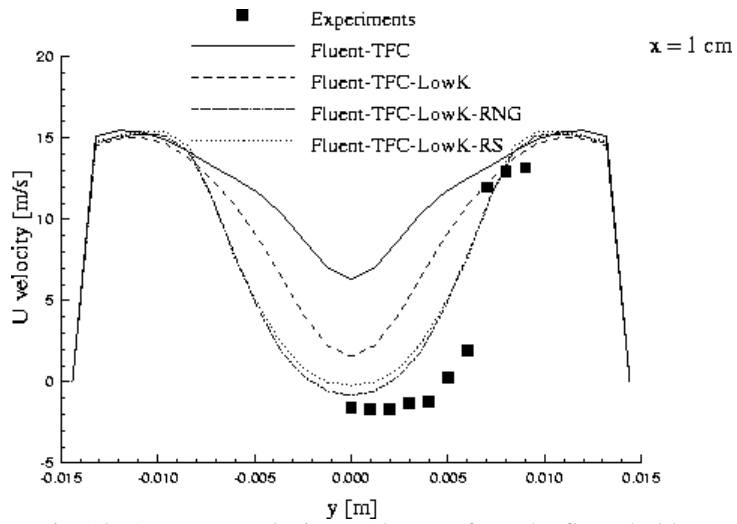Fig. 9: Turbulent kinetic energy profiles at 10 [mm] from the flame holder.

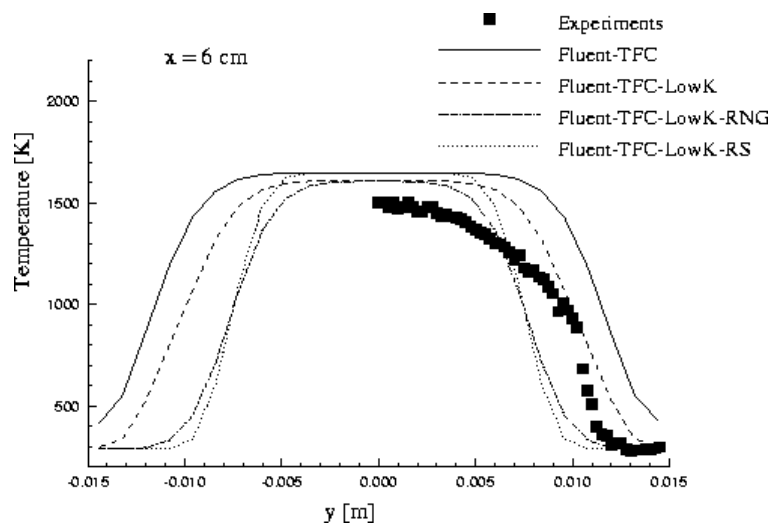Fig. 10: Average x-velocity at 10 [mm] from the flame holder.

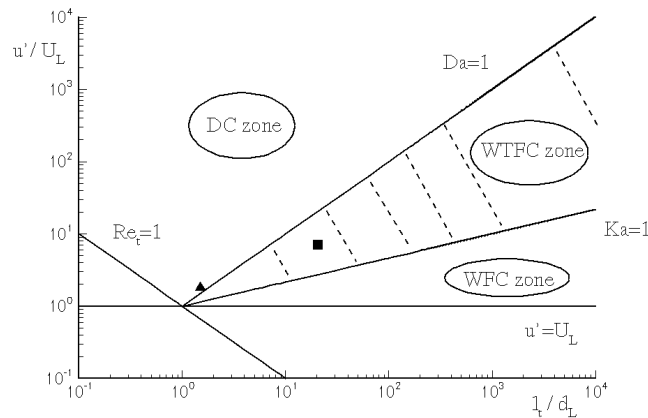Fig. 11: Average temperature profiles at 60 [mm] from the flame holder.

Fig. 12: Borghi's diagram: ▲ENSMA working point, ■ Moreau working point; (combustion regimes: DC = distributed; WFC = wrinkled flamelets; WTFC = wrinkled-thickened flamelets); u': turb. intensity; U_L: lam. flame speed; l_t: turb. integral length scale; d_L: lam. flame thickness

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