# Validation of a new chemistry reduction method for partially-premixed laminar methane/air flames.

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## 1 Introduction

Partially-premixed laminar flames are of great importance for domestic burner manufacturers. They represent the most attractive solution to cope with the latest pollutant emission regulations. To improve our knowledge of this kind of flame, numerical simulations are very useful. But these simulations remain too costly when one needs to consider the full complexity of the chemistry. In fact, in order to correctly describe a laminar flame, it is very important to accurately represent all the phenomena (convection, diffusion and reaction) throughout the flame front. That is why we need to use detailed chemistry mechanisms instead of single-step chemistry. Unfortunately detailed mechanisms include more than fifty species and hundreds of reactions in the case of methane/air flames.

A solution to overcome this problem is to use reduced mechanisms. There are different ways to generate these mechanisms. The classical technique is based on physical assumptions (steady state and partial equilibrium..., Peters 1985). This technique gives good results but requires an impressive knowledge in chemistry and is very costly in terms of human time. As industrials can not afford such a solution, researchers have more recently developed fully automatic techniques to provide reduced mechanisms. Maas and Pope (1992) proposed a reduction technique, called ILDM, based on the study of the chemical local time scales. More recently, the Flame Prolongation of ILDM (FPI) method, a new improvement, was proposed (Gicquel et al. 2000). Its main advantage is that the description of the low-temperature phenomena is based on better physical assumptions.

In the present work, this technique is used to compute partially-premixed laminar flames. To validate the FPI technique, three test-cases were simulated in the TOPDEC burner configuration (Perrin et al. 1998). The TOPDEC burner is an idealised partially-premixed laminar burner which is developed in an European Community project. Simulations were compared to OH and temperature measurements.

This article is structured as follows: we first give a short description of the FPI method. Then the TOPDEC configuration and the experimental setup are presented. We afterwards describe the numerical simulations performed in three different configurations and the comparison with experimental results.

## 2 The FPI technique

The FPI technique is an improvement of the well-known ILDM method. For further details on ILDM see Maas and Pope (1992). The original ILDM is able to accurately reproduce the high temperature phenomena. But the low-temperature ones are described with a linear prolongation between the fresh gases and the high temperature zone. This linear prolongation introduces some discrepancies, which lead to errors close to 100% on the laminar flame speed prediction for a methane/air flame, with a two-dimensional manifold.

As our goal is to apply this technique to laminar combustion simulations, we have to use a model which gives a good estimation of the laminar flame speed as well as the low temperature region of the flame. That is why we propose a new extension of the ILDM technique called FPI. The FPI method consists of using the part of the chemical state space accessed by a one-dimensional freely propagating flame in order to extend the corresponding one-dimensional ILDM manifold in the low-temperature zone. This method is detailed in Gicquel et al. (2000) and has already been validated for premixed counterflow hydrogen/air flames. Our aim in this work is to validate it now for partially-premixed methane/air flames.

For the present simulations we use an FPI look-up table based on a methane/air mechanism. This detailed mechanism was proposed by Lindstedt (1998). It includes 30 species and about 300 reactions. The look-up table is constructed with two variables as coordinates which are $CO_2$ for the chemistry and $N_2$ to take into account the mixing effects.

The look-up table can be used for equivalence ratios comprised between 0 (pur air) and 1.7 (extinction limit). This look-up table includes 6550 grid points. Its generation was fully automatic and has been done in about an hour on a Sun Ultra 5 workstation.

## 3 TOPDEC reference test-cases

The TOPDEC burner presented in figure 1 is an idealised domestic boiler employing a 2D partially-premixed laminar burner (Perrin et al. 1998). Its power input is equal to 10 kW. This burner is similar to commercial ones with the difference that the primary and the secondary air flowrates are independently adjustable and full optical access is available.

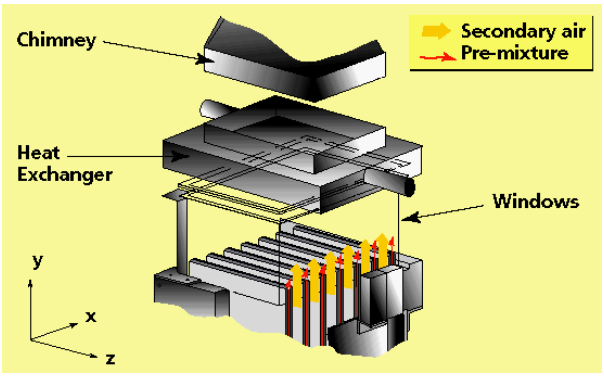



Figure 1: TOPDEC burner configuration

Different measurement techniques have been used. In this paper we will present results obtained with thermocouple measurements for the temperature fields (Miquel et al. 1998). These results are used to validate global information concerning the flame. It is not recommended to use them to deduce any information about the flame front position because the thermocouple (4mm diameter) induces lots of perturbations in the flame shape (intrusive method). In order to check the flame front position, we compare the OH profiles obtained numerically and with Planar Laser-Induced Fluorescence on OH (Brenez et al. 2000).

Three different cases are used to validate the FPI technique. All cases have the same global equivalence ratio ($\phi$ = 0.71). The first one (Case 1) is a locally rich partially-premixed laminar flame ($\phi_p$ = 1.667) (see table 1). Cases 2 and 3 correspond to locally lean ($\phi_p$ = 0.8314) partially-premixed flames. The difference between them is that in Case 3 an insert is added in the middle of the injector. This insert has a great influence on the flame stabilisation.

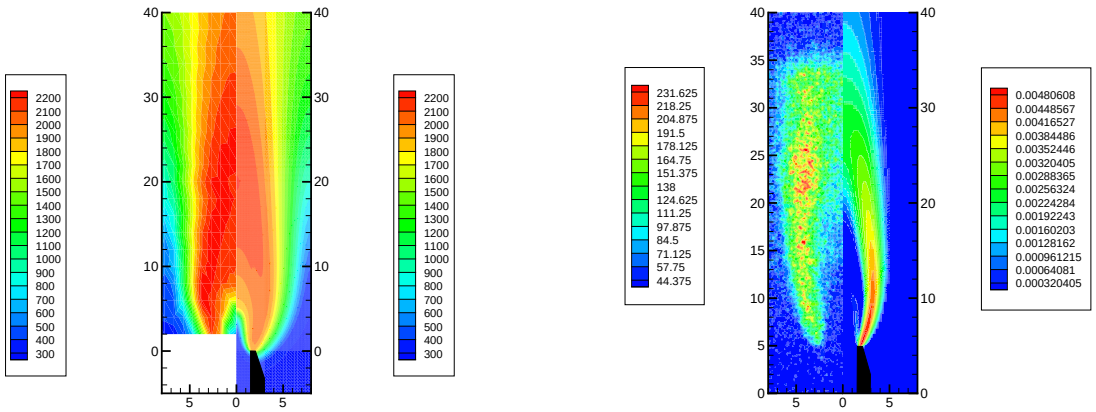
| case | 1 | 2 | 3 |
|---|---|---|---|
| $\phi_{\text{primary}}$ | 1.667 | 0.8314 | 0.8314 |
| primary inlet velocity (m/s) | 0.4731 | 0.9776 | 1.4500 |
| secondary inlet velocity (m/s) | 0.2042 | 0.0510 | 0.0510 |

Table 1: Description of the three test-case inlet boundary conditions used in this paper

The numerical simulation relies on a mesh including 15 000 cells. The smallest cell size is $80\mu$m $\times$ $80\mu$m. As we solve only relatively smooth species ($N_2$ and $CO_2$), that is small enough. If we had to use a detailed mechanism we might have to use cells smaller than $10\mu$m $\times$ $10\mu$m to solve correctly all the radicals inside the flame front. With the FPI technique these radicals as well as temperature are obtained only by reading in the look-up table using $N_2$ and $CO_2$ (Gicquel et al. 2000).

## 4 Results and Discussion

The temperature comparison performed in Case 1 (Fig. 2) shows a good agreement between experimental and numerical predictions. Both the maximum value and the global distribution of the temperature are well predicted by the FPI method. The OH mass fraction which characterises the diffusion flame position is also well predicted (Fig. 2). The temperature field shows a flame front right after the primary inlet. But as the primary mixture is rich ($\phi_p$ = 1.667), the unburned gases react with the secondary air forming a diffusion flame which can be clearly observed on the OH field. In Cases 2 and 3 in contrast with Case 1, the primary



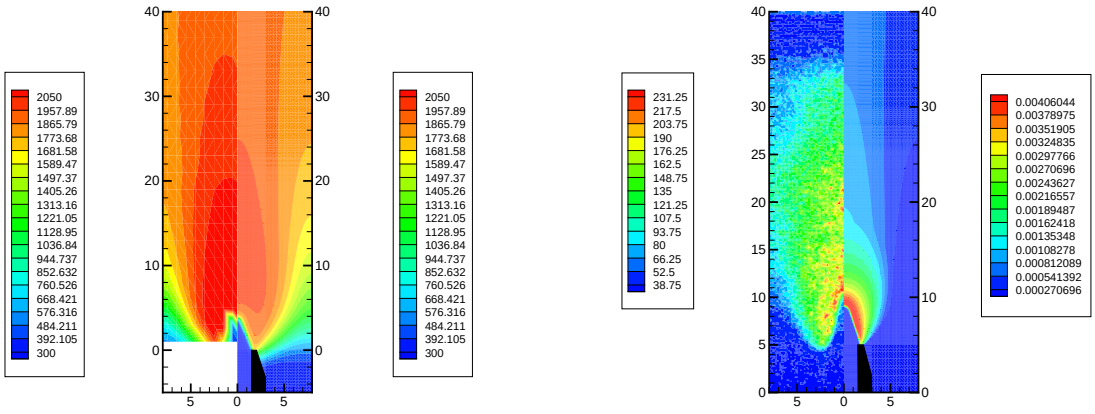

(a) Temperature

(b) OH

Figure 2: Comparison of experimental (on left part of each graph) and numerical (on the right) results for Case 1.

mixture is lean. There is no diffusion flame. In Case 2, the flame is characterised by the typical Bunsen-type flame shape (Fig. 3), while in Case 3 the introduction of the insert induces a butterfly-type flame shape (Fig. 4). This change of shape is well reproduced by the numerical simulations.

The flame position in Case 2 is correctly estimated (Fig. 3). The small difference is due to the adiabatic walls used for these simulations. Figure 4 shows that the butterfly shape of the flame is well predicted as




(a) Temperature

(b) OH

Figure 3: Comparison of experimental (on left part of each graph) and numerical (on the right) results for Case 2.

well as the angle of the V profile. This very sensitive phenomena induced on the flame shape by the addition of the insert is perfectly predicted by the FPI method. This shows that all the effects of the chemistry are perfectly taken into account with the FPI reduction technique.

All these simulations were performed with the commercially CFD code ESTET (Matthei and Simonin 1993) using the FPI package developed for this study. They were performed on a standard workstation and required less than 3 hours of CPU time each. This computational time is fully compatible with industrial requirements.

## 5 Conclusion

In this paper, we applied the FPI technique to three different partially-premixed laminar flames. One was locally rich and two were lean with a difference in flame shape. The FPI technique was able to reproduce all the operating points of an industrial laminar burner. The position and shape of the flame are perfectly predicted as well as the temperature field. As we use a table look-up, it is also possible to obtain accurately all the other species (these results will be presented in the full paper).

The computational time needed was about 3 hours on a standard workstation using a commercially-available CFD code. This small CPU time will allow a larger usage of numerical simulations in the conception process of new burner designs.

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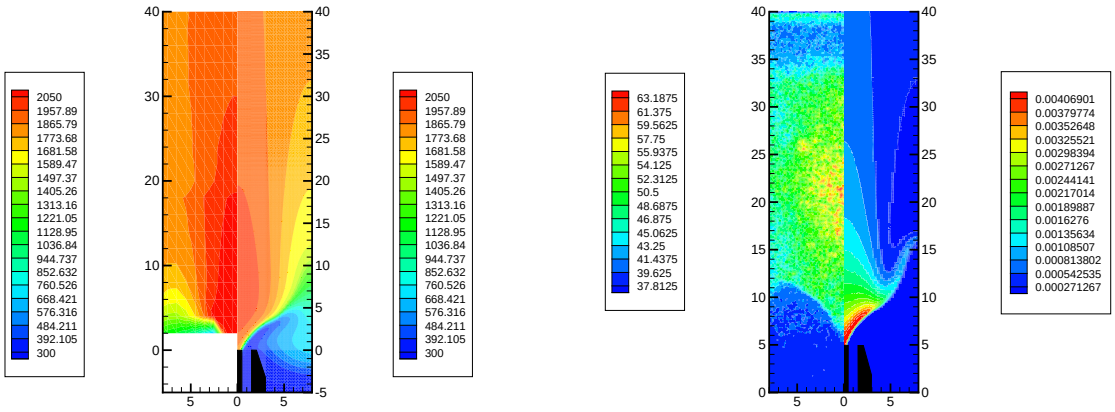


(a) Temperature

(b) OH

Figure 4: Comparison of experimental (on left part of each graph) and numerical (on the right) results for Case 3.


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