Fast and Accurate Flame Computations Using Detailed Chemistry and Transport

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1 Introduction

Accurate simulations of flames and of their detailed structures are important from scientific, economical and ecological points of view: they are needed for fundamental research in order to improve the knowledge about laminar flame structure but also for industrial applications, since manufacturers of domestic burners have to cope with drastic regulations on pollutant emissions. Unfortunately, these simulations remain at present time very costly and everything must be done to cut down computing times.

We have developed a powerful combustion code for 2D and 3D gas flame computations, using efficient numerical methods and an elaborate physical interface including different levels of accuracy. Detailed models are available to describe chemistry and diffusion, but it is also possible to use simplified, reduced models for faster simulations. With a view to meet the requirements of the gas burner industry, a low-Mach number approximation is used in order to circumvent the usual CFL restriction.

In the first part of this paper we emphasize the main features of the code and its numerical methods. The second part describes the physical interface to detailed and reduced models. In the last part we show some results obtained with detailed chemistry and transport as well as a comparison with experimental measurements for validation purposes.

2 The UGC$^+$ code

Our simulation code is named *UGC*$^+$ (Paxion et al. 2000; Baron et al. 2000) and is based on the *UG* multi-purpose library (Bastian et al. 1997). It uses multi-level conforming unstructured grids on 2D or 3D domains, with a cell-vertex finite-volume discretization. This discretization is second order in space. Dynamic local refinement and coarsening functions

make it possible to adapt dynamically the grid during computations, with regard to physical or computational criteria.

Low-level parallel routines using efficient load-balancing algorithms enable the code to run on distributed memory supercomputers (e.g. Cray T3E) or PC clusters. Local multigrid cycles can be performed as a preconditioner for linear iterative solvers, resulting in higher convergence rates. At the top of the multi-level object-oriented structure of the code, an advanced command interpreter allows the user to edit interactively the computation parameters during run time.

The code evolves by time-marching, and the time-step is automatically adapted during computations according to global convergence results. The time discretization is first-order and implicit. Fixed point or approximate-Newton iterations achieve the linearisation of the Navier-Stokes and thermo-reactive equations and a Bi-CGSTAB algorithm, preconditioned by multigrid V-cycles with Gauss-Seidel or ILU smoothers, solves the resulting linear system. These numerical methods take advantage of the sparse structure of the Jacobian for storage and computations (Neuß 1999).

3 The physical interface

We have implemented a complex physical interface coupled to several packages to provide the chemical and diffusional terms involved in the governing equations. In order to enable accurate computations, detailed models are included, thanks to the *CHEMKIN II* (Kee et al. 1991) and *EGLIB* (Ern and Giovangigli 1997) libraries.

These routines use detailed reaction schemes involving many chemical species and reactions. As a result, they imply a high computational cost, since each chemical species mass fraction is an unknown in the system. Moreover, the use of detailed models results in stiff equations that need to be solved on very fine meshes with small time-steps.

Recently, a new sub-interface has been developed in UGC^+ to *FPI* routines. The *FPI* (Flame Prolongation of *ILDM*) method (Gicquel et al. 2000) is an extension of the well-known chemistry reduction *ILDM* method (Maas and Pope 1992), with a prolongation to low-temperature zones using 1D flames. With this method all the chemical and diffusional terms involved in the equations can be pre-tabulated in a look-up table, as functions of two coordinates (one for the chemistry and the other to take into account the mixing effects).

Consequently, instead of solving as many equations as species in the chemical scheme, only two transport equations are required for the whole thermo-reactive part of the system. Moreover, these equations are easier to solve and coarser meshes as well as larger time-steps can be used. Thanks to the *FPI* method, we hope to decrease the computing times by one order of magnitude at least compared to detailed simulations.

If the main interest is on fast computations, the *FPI* routines can be sufficient. If more accurate solutions are needed, the *FPI* results are used as a (very good) initial guess to initialize detailed computations.

4 Results on the Topdec configuration

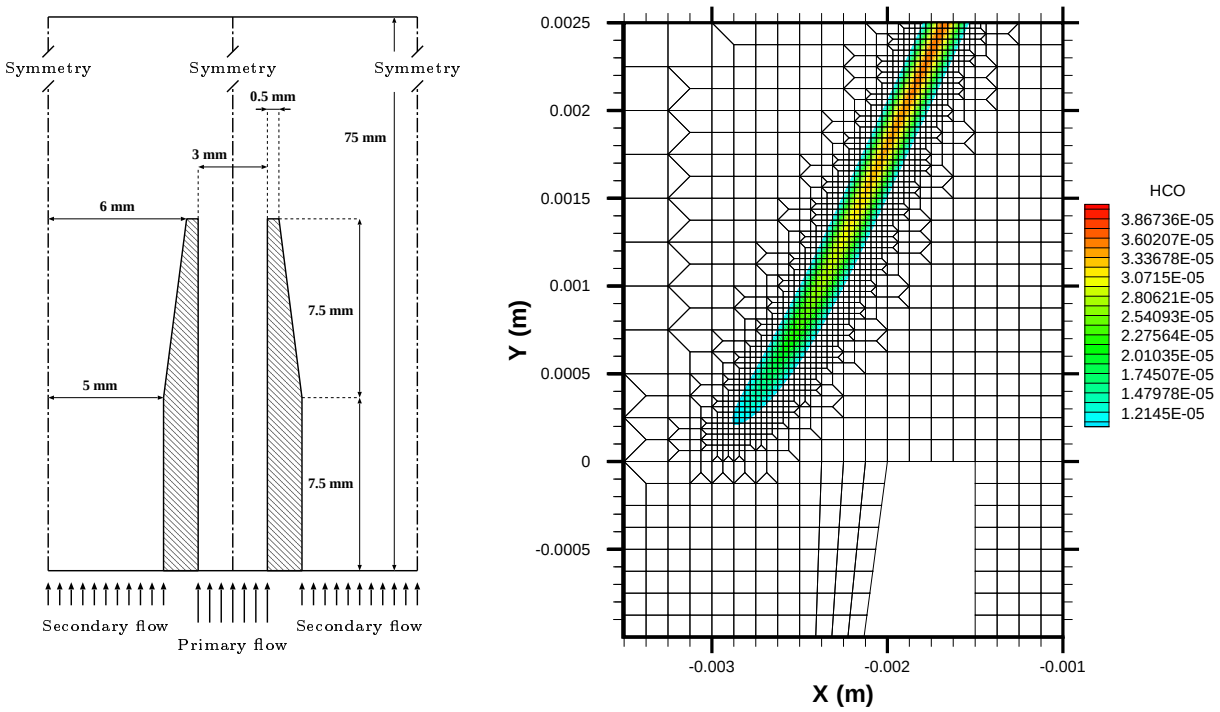

Figure 1: Computational configuration for the *Topdec* burner (left). The final multigrid structure uses 5 levels and 15200 surface nodes. Close-up on the injector tip showing conforming local refinement, and the HCO mass fraction (right). The elements on the finest level are about 30 μm large.

We present some results obtained with detailed chemistry and transport on an idealized boiler configuration: the *Topdec* burner (Perrin et al. 1998).

The experimental burner consists of seven rows of two-dimensional injectors, which, for the middle injector, can be approximated by an infinite number of injectors. It is therefore possible to reduce the computational domain to half an injector and symmetry boundary conditions (FIG 1). The primary flow is a lean methane/air mixture, with an equivalence ratio of 0.83, injected at 0.98 m.s^{-1}. A secondary air flow is injected between the primary injectors at 0.05 m.s^{-1}. The global equivalence ratio is 0.71.

The full computation starting from a very rough initial solution takes about 20 hours on a SUN Ultra-5 workstation with a final surface grid of about 15200 nodes (FIG 1).The reaction scheme consists of 14 chemical species and 37 reactions (Coffee 1984). Results show good agreement with experimental measurements in the flame front, for temperature, CO_2 and OH (FIG 2).

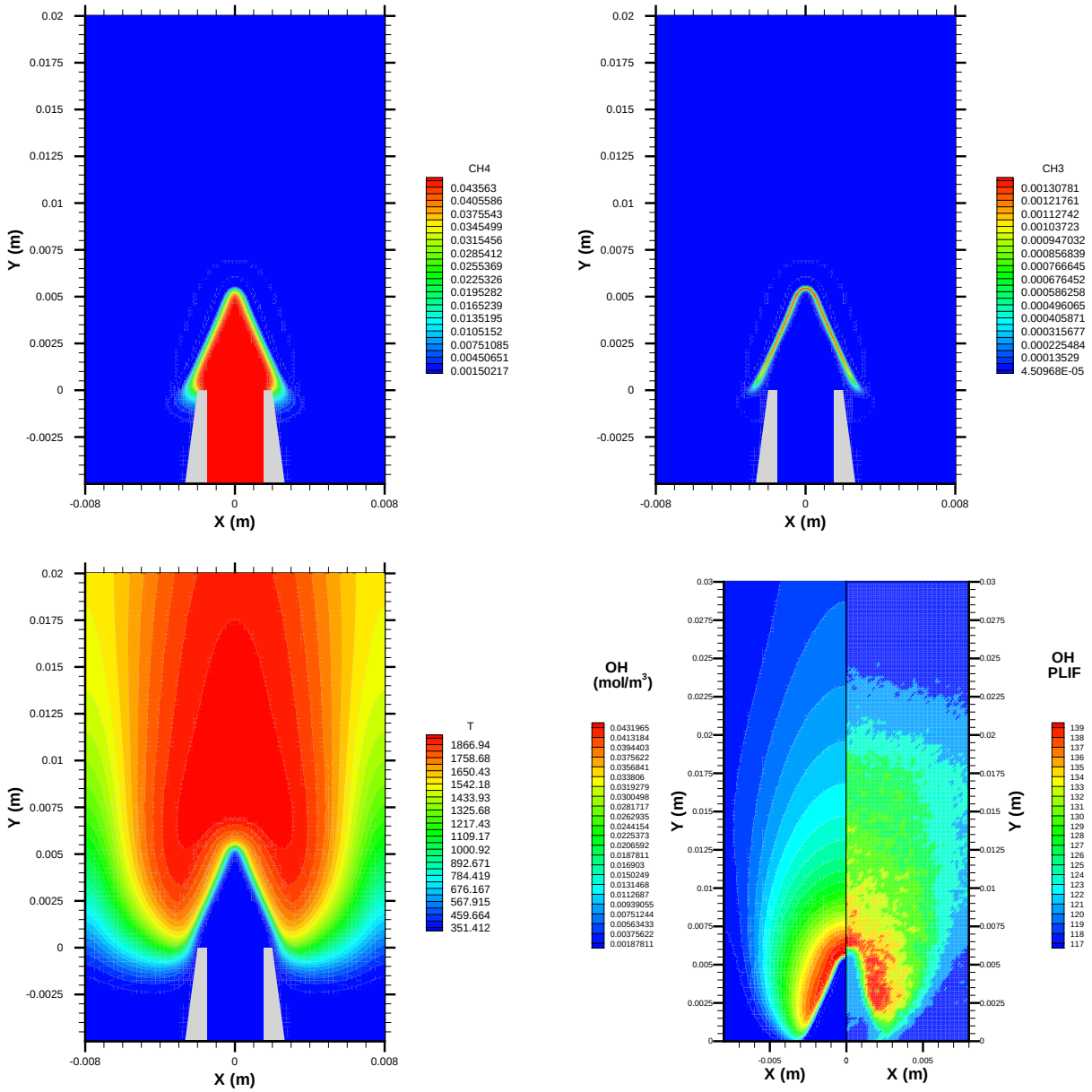

Figure 2: Results of the *Topdec* computations. CH_4 (top-left) and CH_3 (top-right) mass fractions and temperature (bottom-left), obtained by numerical computation. In the bottom right-hand corner, comparison on the OH species between computed molar concentration (left) and experimental results (Planar Laser Induced Fluorescence, right).

5 Conclusion

The *UGC*$^+$ combustion code we have developed offers the possibility to use both detailed and reduced models for chemistry and diffusion, combined with powerful numerical methods.

Good results have already been obtained with detailed chemistry and transport starting from a rough initial solution.

In the near future, the implementation of the *FPI* method will enable much faster computations. Thanks to the expected speed-up, we will tackle new applications using UGC^+. We will first carry out real 3D computations (first tests have already been computed). An effort towards automatic optimization of gas burners will be performed at the end of this year. Finally, unsteady simulations will be carried out in order to demonstrate the possibility of using UGC^+ for turbulent flames, in particular in the frame of Large-Eddy Simulations.

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