Finite rate chemistry effects and combustor liner heat transfer studies in a framework of LES of turbulent flames

- investigation of pollutant formation using OpenFOAM

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Abstract

At The Hong Kong Polytechnic University, the OpenFOAM tool box has been used to simulate a variety of academic combustion and heat transfer problems as well as problems relevant to industrial situations. The use of a common and wide spread CFD code has also been a strong common ground and enabled to start cooperation across the globe (Sweden and Denmark). Further, OpenFOAM ensures high scientific quality as conducted numerical experiments are easily repeatable for other researchers.

The authors have developed a low Mach number large eddy simulation (LES) solver for the application of finite rate chemistry to flame simulation. We stress here that the tool was tailored for using efficiently relatively large mechanisms far beyond the traditional 1 and 2-steps approaches. The advances offered by the skeletal mechanisms open new avenues for simulating flames especially non-adiabatic or near extinction/piloted flames. A number of cases have been studied, based on two different setups. The first setup is a piloted premixed jet flame with strong finite rate chemistry effects present, which is being used as a target case for validation of the solver. The jet flame was studied experimentally in [1], and thorough experimental data is available, covering velocity, temperature, and species. Boundary conditions are well prescribed, which together with the detailed measurements make the flame an ideal challenging test case for CFD. Also, the flame is stabilized by a mechanism which is similar to gas turbine conditions. The setup consists of a central jet pipe with a diameter of 4 mm which issues a methane/air mixture at a relatively high speed. The central jet is surrounded by a pilot consisting of hot product gases being issued at a low velocity. Reactions are mainly taking place in the shear layer between the jet and the pilot. Given the strength of the shear, the reaction zone is subject to strong turbulent mixing rendering a global Damköhler number of about 0.01 and a Karlowitz number of about 1600. This places the flame in the distributed reactions regime where effects of the finite reaction rate are significant. We should point out that this particular flame regime has not been investigated in details so far. Indeed a very large fraction of the published data covers the so-called *flamelet* regime which is easier to access in laboratory experiments and also easier to model. When departing from the *flamelet* regime, finite rate chemistry effects become non-negligible as pointed out in [1] but until recently this regime was not being investigated. It is important that OpenFOAM enables investigation that is at the forefront of combustion research and also emulates cooperation where a common CFD tool and the open-source culture favor exchanges.

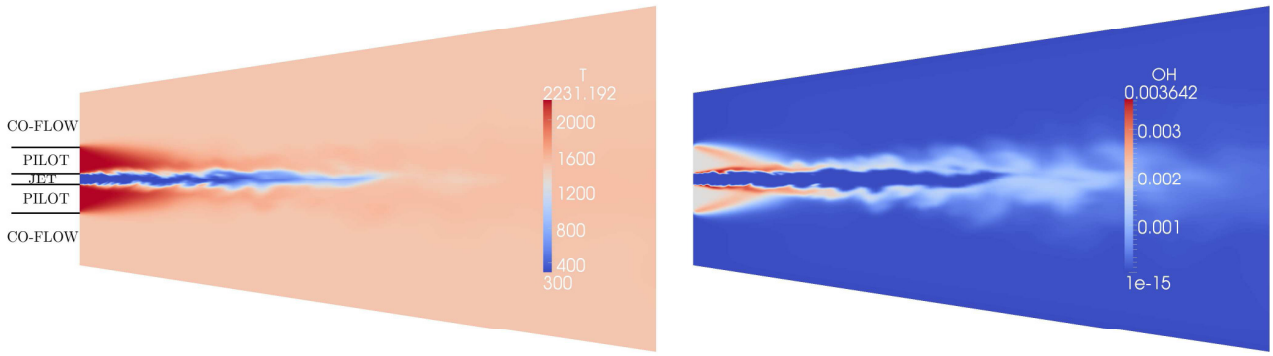

Fig 1. Left: a snapshot of the temperature field from the jet flame simulation. A central jet issues a lean methane/air mixture at a bulk flow rate of 100 m/s. Surrounding the jet is a pilot consisting of product gases from a stoichiometric methane/air flame at a bulk flow rate of about 5 m/s. The pilot, in turn, is surrounded by a co-flow of product gases from a lean hydrogen flame. Right: A snapshot of the hydroxyl radical concentration field.

A number of simulations have been carried out to assess influences of mesh resolution and choice of reaction scheme. As the complexity of the chemistry is becoming increasingly important at low Damköhler and high Karlovitz number, one would expect to see benefits of larger, more complete, reaction schemes. Indeed, this is also observed as temperature and species concentration fields are being compared with experimental data in Fig. 2. Generally it can be concluded that the more complex the mechanism the better the results. Particularly CO is important to predict successfully, as it causes significant pollution, and also poses challenges in modeling due to sensitivity to heat losses.

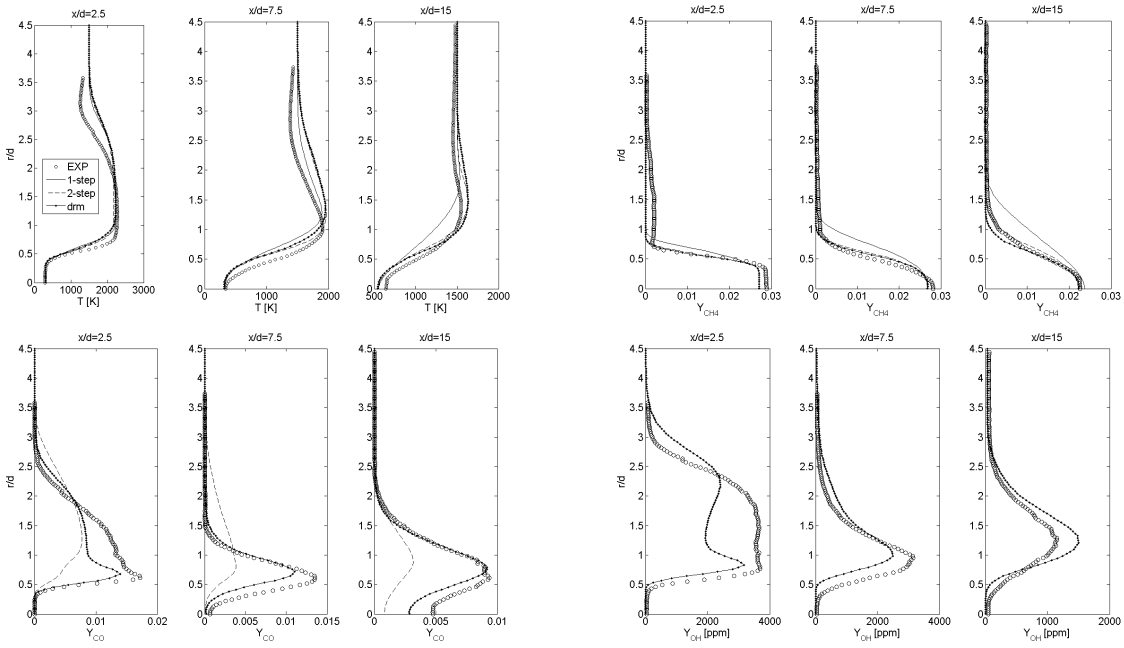

Fig 2. Radial profiles of temperature and mass fractions of methane, carbon oxide, and the hydroxyl radical at different axial positions. Results from experiments and from three computed cases applying different levels of reaction complexity. The experimental data were kindly provided by M. Dunn (Sandia National Laboratories).

The second setup is based on a swirl burner, which was constructed in Hong Kong. The burner, Fig 3, was designed to allow for a wide range of swirl numbers and flame configurations reproducing a wide range of conditions that are relevant to industrial devices. A well chosen set of operation conditions were experimentally quantified with PIV performed at Lawrence Berkeley National Laboratory. In a case study, the influence of confinement on the flow and flame was addressed. While keeping the burner conditions constant, PIV was performed with and without a confinement emulating a typical gas turbine combustor, in particular with a strong outlet contraction. These two conditions were investigated using the newly implemented solver, firstly for validation and secondly for providing further insight into the flame stabilization and heat-losses at the combustor walls.

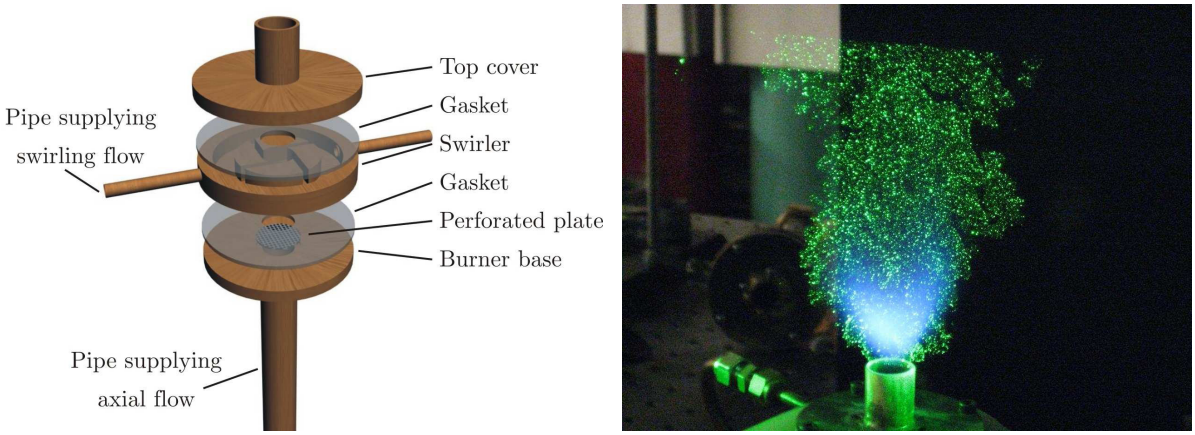

Fig 3. Left: The swirl burner in an exploded view. Separate supplies for swirling and non-swirling flow are used to control the level of swirl. Right: The burner in operation with a green light sheet illuminating the seeding and the blue light from the detached and lifted U-shaped flame.

Results show that the confinement effects are manifested in the downstream and lateral regions of the flame while the central region near the burner exit is relatively unaffected, Fig 4. As can be observed, the temperature fields of the open and confined flame differ substantially due to entrainment of surrounding air by the unconfined flame in the farfield. The same significant change on the visible flame was however not observed experimentally. The visible flame had a U-shape under both confined and unconfined operation conditions, while the visible flame of the simulated cases in Fig 4 would have a U- respectively an M-shape. The simulation shown in Fig 4 was done under adiabatic conditions, while experiments were carried out under conditions where the wall temperature of the combustor was much lower than the adiabatic flame temperature. Under adiabatic conditions, the fluid remains at a constant temperature in the post flame zone throughout the combustor.

Fig 4. The mesh with a cross section showing a snap shot of the temperature field. Left: the case with the unconfined flame, and right: the confined flame.

To address the potential influence of heat losses to the combustor walls on the flame shape, a new mesh, with a y^+ of about 2, capable of capturing heat transfer was created. Further, a skeletal mechanism capable of accurately capturing quenching and re-ignition was engaged. Wall temperature was measured experimentally and fed to the simulation, and, indeed, a different flame shape is observed. Figure 5 shows a snap shot of the temperature field from the non-adiabatic simulation. Substantially lower temperatures are seen in the corner recirculation zones and the shape of the reaction zone resembles more the shape of the reaction zone for an unconfined flame. Given the capabilities of OpenFOAM to address conjugated heat transfer, a future activity could be to also solve for the temperature evolution in the combustor walls.

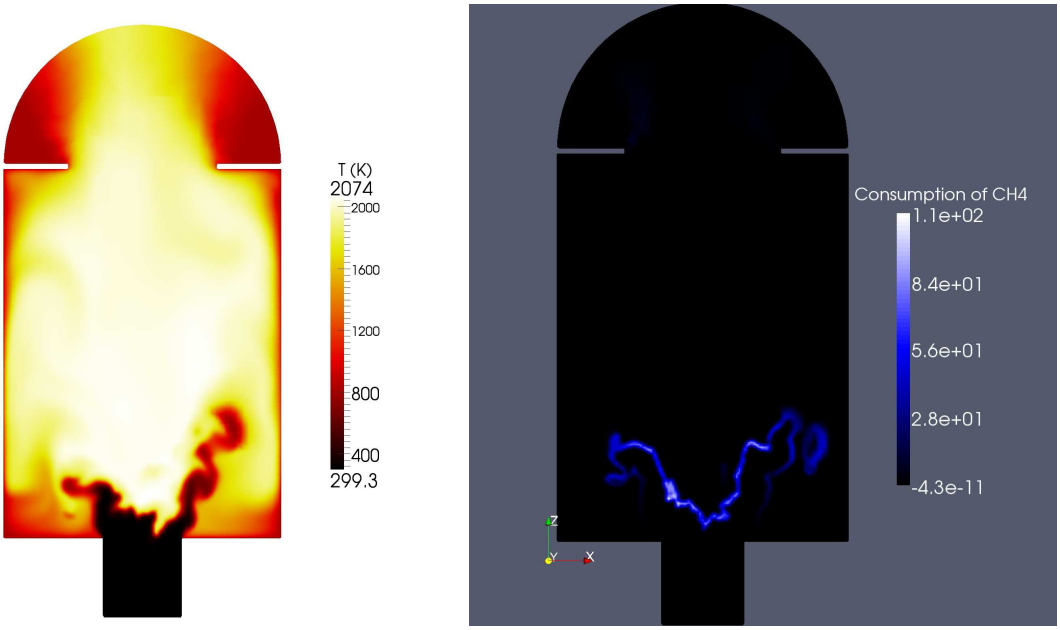

Fig 5. Left: A snap shot of the temperature field from the simulation with realistic wall temperatures. Right: A snap shot of the consumption rate of methane (not from the same time step), now having more of a U-shape.

Key words: Finite rate chemistry, heat transfer, large eddy simulation, detailed chemistry modelling

References

[1] M.J. Dunn, A.R. Masri, R.W. Bilger: *A new piloted premixed jet burner to study strong finite-rate chemistry effect*, Combustion and Flame 151, pp. 46-60, 2007