DETAILED HOMOGENEOUS AND HETEROGENEOUS KINETICS IN OPEFOAM

ALBERTO CUOCI[1], MATTEO MAESTRI[2]
[1]*Dep. of Chemistry, Materials, and Chemical Engineering, Politecnico di Milano, alberto.cuoci@polimi.it*
[2]*Dep. of Energy, Politecnico di Milano, matteo.maestri@polimi.it*

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Today it is well recognized that realistic numerical simulations of reacting flows require not only accurate, detailed modelling of fluid dynamics, but also a detailed description of chemical reactions and physical and chemical properties of gas mixtures. In particular, the inaccuracy of simplistic approaches assuming either equilibrium chemistry or global mechanisms has been clearly demonstrated, especially in combustion. In heterogeneous catalysis the superior predictive capabilities of microkinetic mechanisms are today commonly accepted.
This has led to an increasing effort to develop and incorporate more complex reaction mechanisms in the numerical simulation of multidimensional reacting flows. The result is the availability of a huge number of kinetic mechanisms with different levels of detail and comprehensiveness. Sufficiently realistic, comprehensive kinetic mechanisms describing pyrolysis, oxidation and combustion of hydrocarbon fuels usually consist of hundreds of species and thousands of reactions. Obviously, the number of species and reactions increases with the complexity and the size of the fuel molecule. As an example, if the largest kinetic mechanism for n-heptane involves ∼600 species and ∼3000 reactions, the oxidation of methyl-decanoate, a methyl-ester used as a biodiesel surrogate, is described by a mechanism with ∼3000 species and ∼9000 reactions [1].
Nevertheless, the coupling of CFD with detailed kinetic mechanisms for combustion and/or with microkinetic models for heterogeneous reactions represents a very challenging problem, due to the potential huge number of chemical events and species in the gaseous phase and/or along the catalyst and the wide range of spatial and time scales introduced by the reactions. This results in severe demands on computational resources, especially because of the large number of highly non-linear, stiff equations to be solved. Moreover, the spatial discretization has to be sufficiently fine to properly describe the high gradients of density, temperature, and composition close to the flame front and/or along the catalytic surface. Therefore, the numerical modelling of multidimensional reacting flows with realistic homogeneous/heterogeneous kinetic mechanisms can be considered a challenging problem and poses strong requests on the computational resources. The resulting memory requirements and the computational efforts (i.e., the CPU time) are significant and often prohibitive. In particular, conventional CFD methods, based on purely segregated algorithms, cannot be efficiently applied in this context, since they have serious difficulties to treat the stiffness and the high non-linearities of the equations. The counterpart would

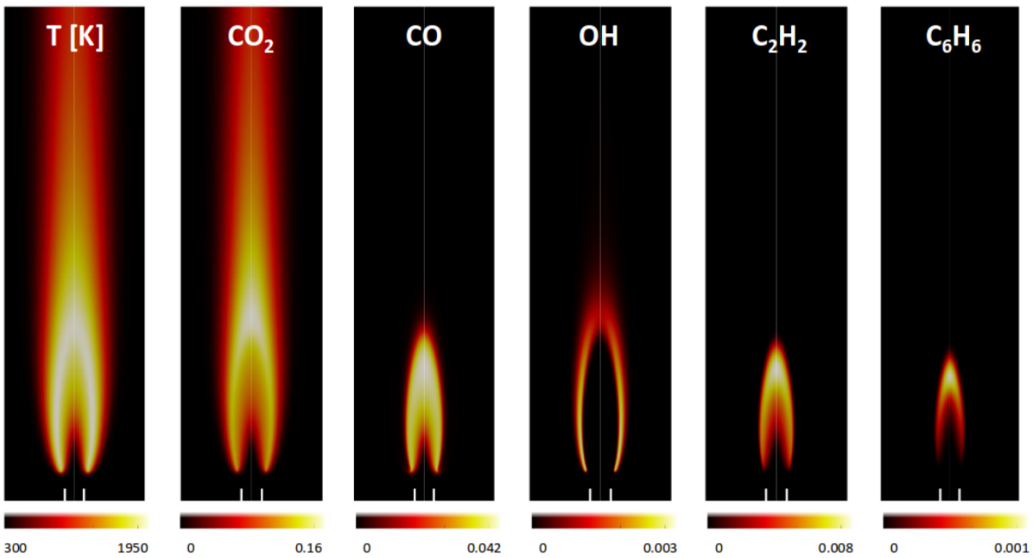

Figure 1: Lifted coflow laminar diffusion flame fed with methane: calculated temperature [K] and mass fractions of selected species

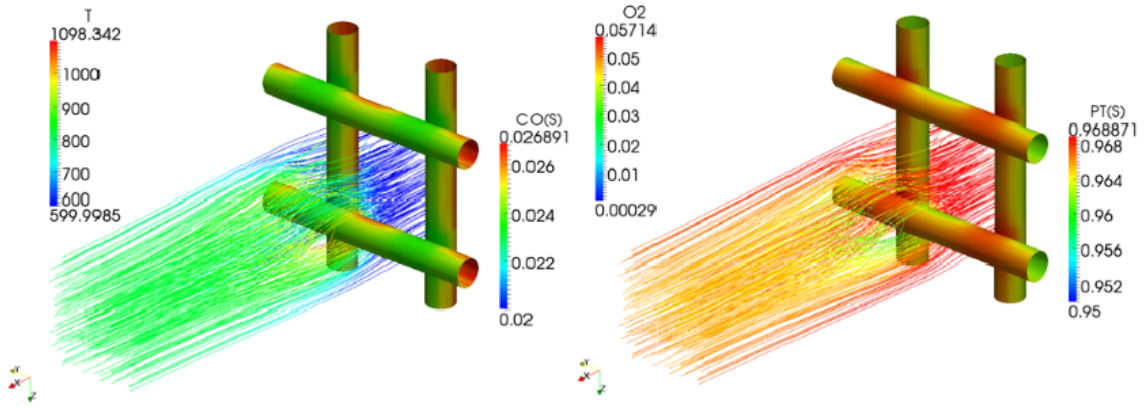

Figure 2: Catalytic Partial Oxidation (CPO) of methane over a platinum gauze: calculated temperature [K] and mass fractions of selected species

be the application of fully-coupled methods, but these algorithms can be applied only to relatively small systems.
In order to overcome the issues reported above, we recently implemented in OpenFOAM the so called "operator-splitting" approach for the efficient coupling between detailed kinetic mechanisms and CFD [2, 3]. In recent years, operator-splitting methods have been widely applied in reactive flow calculations, especially for combustion problems and atmospheric modelling studies. The main advantages are that (i) many costly matrix operations (typical of fully coupled algorithms) can be easily avoided and (ii) the best numerical methodology for each type of term or process can be chosen among several possibilities. extended the technique, usually proposed only for homogeneous chemistry, to heterogeneous catalytic processes. The proposed OpenFOAM-based code was developed with the aim to efficiently perform CFD simulations for very general geometries, with arbitrarily complex homogeneous/heterogeneous kinetic mechanisms. The code can be used for steady-state and unsteady flows in complex grids.
The proposed code was applied to simulate several reacting flows with different degrees of complexity, under both steady-state and transient conditions. In particular, simulations of coflow diffusion flames with detailed mechanisms (300 species) in 2D were successfully performed to study the formation of carbonaceous particles (soot). Good agreement with published experimental data for was achieved. The code was also adopted to study 3D randomly packed beds using UBI/QEP microkinetic models to account for the surface reactivity.
The quality of the solver was further measured by analysing its performance on multiprocessor architectures. The code showed a reasonable scalability up to $\sim$100 processors (with parallel efficiency at least equal to 70%) for rectangular, structured meshes, which can be considered a good result, especially considering the generality of the code and the possibility to apply it to arbitrarily complex geometries. More interestingly, as already observed in [4], the parallel scalability increases with the number of species in the adopted kinetic scheme was confirmed. This means that the code can be considered an ideal platform for the numerical simulation of combustion systems with very detailed kinetic schemes.

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