

NUMERICAL MODELING OF LAMINAR COFLOW FLAMES WITH DETAILED KINETICS

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Abstract

In this paper a numerical algorithm for the numerical modeling of multi-dimensional laminar flames with detailed kinetic mechanisms is described. The proposed approach is based on the operator-splitting technique, in order to exploit the best numerical method available for the treatment of reacting, stiff processes and transport, non-stiff processes. The algorithm was implemented in the OpenFOAM® framework and was validated for a laminar coflow flame fed with ethylene. The numerical simulations (performed with a detailed kinetic mechanism with ~170 species and ~4800 reactions) showed a satisfactory agreement with the experimental data (temperature and composition along the centerline), demonstrating the feasibility of the suggested methodology.

Introduction

The detailed numerical simulation of multidimensional laminar flames flows with realistic chemical mechanisms represents a challenging problem and places severe demands on computational resources. The numerical description of laminar flames results in a complex mathematical model, because of the large number of chemical species involved and to the characteristics of the flames (presence of high gradient regions, flame fronts, etc). When detailed kinetic mechanisms are used, special attention has to be paid to the numerical algorithms, which must be sufficiently accurate and efficient. In particular, the numerical methods have to be able to manage the resulting set of governing very stiff equations. At the same time, the discretization has to be fine enough to treat the flame fronts and the high gradients adequately. As a consequence, the computational effort in terms of CPU time and memory requirements is considerable and in many cases prohibitive. Conventional CFD methods based on segregated algorithms have serious difficulties to treat the stiffness and the high non-linearities of the governing equations and cannot be efficiently applied in this context [1]. In order to overcome these problems, coupled methods appear to be an attractive alternative. In particular, among others, two main numerical approaches have been used for the resolution of such a stiff system of equations: (i) fully coupled algorithms [2]; (ii) segregated algorithms based on operator-splitting methods [3]. An advantage of fully coupled algorithms is that all the processes are considered simultaneously, so all physical interactions among processes are taken into account together. However, the resulting system of

governing equations can be extremely large (especially when detailed kinetic mechanisms and complex, geometries are considered).

When operator-splitting methods are used, the governing equations are split in sub-equations, usually with each having a single operator, which captures only a portion of the physics present. Splitting approaches can be conveniently applied for the numerical solution of combustion problems, by separating the stiff chemical reaction from the non-stiff transport processes. An advantage of this approach is that it avoids many costly matrix operations (typical of fully coupled algorithms) and allows the best numerical method to be used for each type of process. A disadvantage with respect to fully coupled methods is that separate algorithms can be very complex and usually differ from term to term.

In the present paper the operator-splitting methodology employed by the authors in the detailed numerical simulation of laminar flames is briefly described, together with some details about its implementation in the OpenFOAM® framework [4]. Then, the results deriving from the application of this methodology to the numerical modeling with a detailed kinetic mechanism of a co-flow axis-symmetric laminar C₂H₄/air flame (experimentally studied in [5]) are presented.

Numerical methods

The OpenFOAM® framework [4] is used to solve the usual gas-phase transport equations of continuity, momentum, energy and species mass fractions (not here reported) [3]. The standard OpenFOAM® solver for compressible, unsteady, non-reacting flows (`pisoFoam`) was modified in order to make possible the introduction of detailed kinetic mechanisms. As reported before, an operator-splitting approach, based on the separation of transport and reaction terms, was implemented and is briefly described in the following [6].

For a general transport/reaction system like a laminar flame described by a set of partial differential equations (PDEs), the governing PDEs can be transformed into a set of ODEs by the spatial discretization and the application of the method of lines:

$$\frac{d\boldsymbol{\psi}}{dt} = \mathbf{S}(\boldsymbol{\psi}) + \mathbf{M}(\boldsymbol{\psi}, t) \quad (1)$$

where t is the time, $\boldsymbol{\psi}$ the dependent (or primary) variables (mass fractions and enthalpy), $\mathbf{S}(\boldsymbol{\psi})$ is the rate of change of $\boldsymbol{\psi}$ due to chemical reactions and $\mathbf{M}(\boldsymbol{\psi}, t)$ the rate of change of $\boldsymbol{\psi}$ due to transport processes, such as diffusion, convection, heat loss, inflow/outflow, etc. In order to solve Equations (1) numerically, the time is discretized in increments Δt , and the integration in time is then performed using the so-called Strang splitting scheme [7]. Reaction is separated from the transport process and the numerical integration is performed in 3 sub-steps:

- ✓ **Sub-step 1.** The reaction terms are integrated over a time interval $\Delta t/2$ through the solution of a ODE system:

$$\frac{d\boldsymbol{\psi}^a}{dt} = \mathbf{S}(\boldsymbol{\psi}^a) \quad (2)$$

The initial condition $\boldsymbol{\psi}^a(0)$ is taken equal to the final state $\boldsymbol{\psi}$ from the previous time step and the solution of (2) is indicated as $\boldsymbol{\psi}^a(\Delta t/2)$.

- ✓ **Sub-step 2.** The transport terms (convection and diffusion) are integrated over a time interval Δt by solving:

$$\frac{d\boldsymbol{\psi}^b}{dt} = \mathbf{M}(\boldsymbol{\psi}^b, t) \quad (3)$$

The initial condition $\boldsymbol{\psi}^b(0)$ corresponds to the final state of the system from the Sub-step 1, and the solution of (3) is denoted by $\boldsymbol{\psi}^b(\Delta t)$.

- ✓ **Sub-step 3.** This step is identical to Sub-step 1, with the exception that the initial condition corresponds to the final state of the system from Sub-step 2. The solution is used as the initial condition for the next time step.

It is important to appreciate the mathematical difference between the reaction operator $\mathbf{S}(\boldsymbol{\psi})$ and the transport operator $\mathbf{M}(\boldsymbol{\psi}, t)$. The first is independent of time and does not involve any discretization operation, which means that reaction process is local (separate for each grid point). The transport operator $\mathbf{M}(\boldsymbol{\psi}, t)$ may depend on time if boundary conditions are time dependent; moreover $\mathbf{M}(\boldsymbol{\psi}, t)$ is not separate for different grid points, which are coupled through the gradient in the convective term and the Laplacian in the diffusion term.

Sub-steps 1 and 3 correspond to N independent stiff ODE systems, in $NC+1$ unknowns (species mass fractions and temperature), where N is the total number of computational cells and NC the number of species. Such ODE systems are conveniently integrated over the requested time step using the BzzOde solver [8],

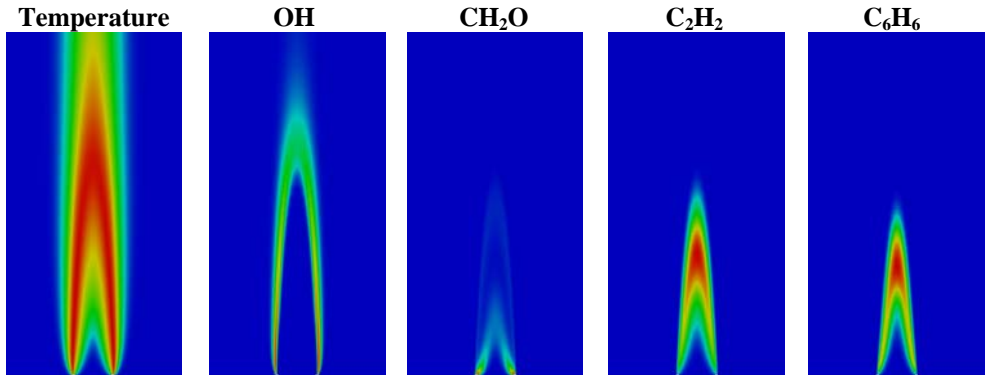


Figure 1. Maps of temperature (max. 1980K) and mass fractions of OH (max. 0.0027), CH_2O (max. 0.0011), C_2H_2 (max. 0.030) and C_6H_6 (max. 0.00105).

which is specifically conceived for very stiff ODE systems arising from the numerical modeling of reactive systems with detailed kinetics. Sub-step 2 correspond to a ODE system of $N \cdot (NC+1)$ coupled equations. However, since these equations are not stiff (the chemical reactions are considered in Sub-steps 1 and 3), the solution is performed in a segregated approach: instead of solving the whole ODE system, $NC+1$ ODE systems are solved, each having dimension equal to N . The continuity and momentum equations are solved in a segregated manner using the well known PISO approach, already available in OpenFOAM® [9].

Numerical results

A coflowing laminar ethylene/air flame has been numerically studied using detailed kinetic schemes. The burner is the same studied in [5].

The numerical calculations were performed on a non-equispaced, structured mesh of 60×80 points, with finest spacing in the region immediately above the burner surface. According to the suggestions reported by Bennet et al. [10], a flat velocity profile was imposed both for the central fuel jet and the coflow stream.

A very general, detailed kinetic scheme, consisting of 167 species and 4744 reactions (POLIMI16HT), was used to describe combustion in the gas phase (the details of the scheme are discussed elsewhere [11]). The kinetic mechanism is available in CHEMKIN format, with the corresponding thermodynamic data and transport properties, at this web address: <http://creckmodeling.chem.polimi.it/>.

Figure 1 reports the calculated maps of temperature and selected species mass fractions. The numerical solutions are compared with the measurements [5]. Figure 2 compares numerical predictions of temperature and main species mole fractions with the experimental data along the axis of the flame. The experimental temperature profile shows a spurious dip at ~ 50 mm because of soot deposition on the thermocouple [5]. The measured and calculated temperatures agree pretty well,

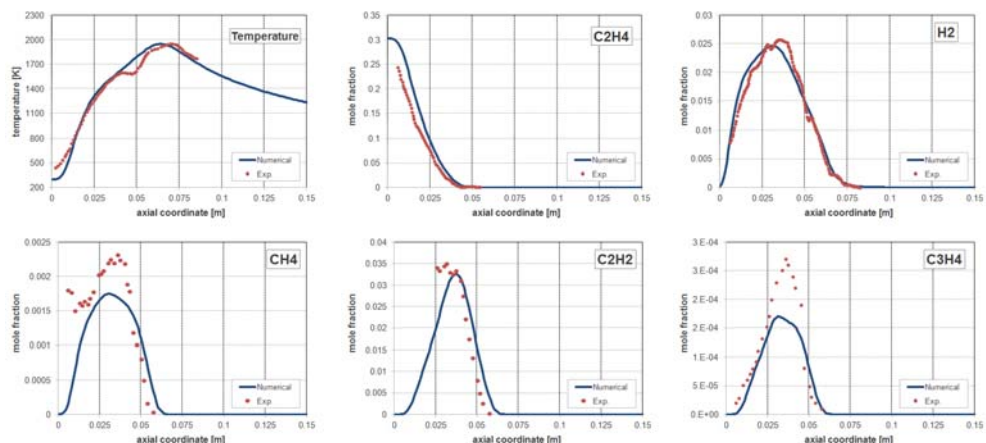


Figure 2. Comparison between numerical predictions and experimental data along the axis: temperature and main species mole fractions.

with the exception of the region close to the central jet nozzle, where experimental values appear 80-100K higher. The temperature peak is located at 67 mm, which is in satisfactory agreement with the experimental value of 71.5 mm. The experimental peak temperature of 1950K was correctly predicted by the numerical simulations, reporting a maximum equal to 1960K. The numerical consumption of ethylene appears slower than experimental data, but this effect is probably related to the preheating effect on the inlet streams. The calculated profiles of O_2 , H_2O and CO_2 are in satisfactory agreement with the measured values. H_2 mole fraction is correctly predicted, both qualitatively and quantitatively. Methane is a little bit underestimated, especially in the region close to the fuel nozzle. The maximum mole fraction of acetylene is predicted quite well, but the peak is shifted to a higher axial location. The model tends to under-predict also the concentration of C_3H_4 isomers (allene and propyne) by a factor of ~ 1.5 .

In Figure 4 the experimental measurements of formaldehyde (CH_2O), benzene (C_6H_6) and naphthalene (C_8H_{10}) are reported against the calculated values, again along the axis. The agreement with the experimental data is quite satisfactory, especially for C_6H_6 and C_8H_{10} . The CH_2O peak is over-estimated by a factor of ~ 1.60 and appears more delayed with respect the experimental data.

The combination of C_2 -radicals with acetylene forms C_4 -species, whose numerical predictions are compared with the experimental data in Figure 3. The model predicts the concentrations of diacetylene (C_4H_2) and C_4H_6 (butadienes and butyne) quite well, together with the peak position, while the concentration of vinyl-acetylene (C_4H_4) is a little bit under-predicted and its peak position shifted towards lower axial position.

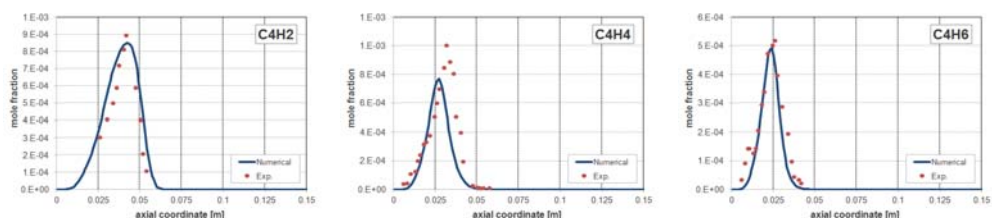


Figure 3. Comparison between numerical predictions and experimental data along the axis: diacetylene (C_4H_2), vinyl-acetylene (C_4H_4) and butadienes + butyne (C_4H_6).

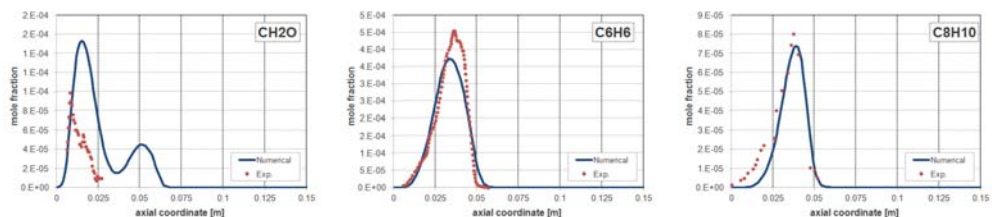


Figure 4. Comparison between numerical predictions and experimental data along the axis: formaldehyde (CH_2O), benzene (C_6H_6) and naphthalene (C_8H_{10}).

Conclusions

In this paper we described the numerical algorithm which was implemented in the OpenFOAM® framework for the numerical modeling of multidimensional laminar flames with detailed kinetic mechanism. The proposed methodology, based on the operator-splitting approach, was validated for a 2D laminar coflow flame fed with ethylene in air. The numerical results were found in satisfactory agreement with the experimental data, demonstrating the feasibility of the operator-splitting approach (coupled with detailed kinetics) for the modeling of reacting flows.

In the future the main task to be accomplished is the improvement of the efficiency of the code: (i) the parallelization of the code for distributed memory architectures; (ii) the implementation of storage/retrieval methods (e.g. ISAT [6]) for the fast numerical integration of Equations (2).

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