XXXIV Evento della Sezione Italiana del Combustion Institute, 24th - 26th October 2011, Rome

Numerical modeling of laminar flames with detailed kinetics

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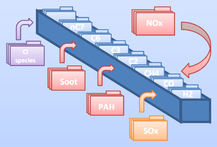
Acknowledgements
Financial support for this activity was provided by the MIUR (Ministero dell'Università e della Ricerca), under the PRIN 2008 framework: "Cinetica dettagliata di formazione di idrocarburi poliaromatici e nanoparticelle da processi di combustione".

Motivation

The detailed numerical simulation of **multidimensional laminar flames** flows with realistic chemical mechanisms is a challenging problem and places severe demands on computational resources. When **detailed kinetic mechanisms** are used, special attention has to be paid to the numerical algorithms, which must be accurate and efficient. 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 equations and cannot be efficiently applied in this context. 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; (ii) segregated algorithms based on **operator-splitting** methods.
When operator-splitting methods are used, the equations are split in sub-equations, with each having a single operator, which captures only a portion of the physics present. Splitting methods can be applied for the numerical solution of combustion problems, by separating the stiff reaction from the non-stiff transport processes. In this work the **operator-splitting** method was implemented in the **OpenFOAM®** framework and applied for the numerical simulation of laminar flames.

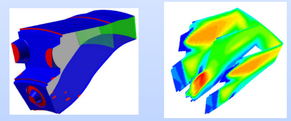
Detailed kinetic schemes



~ 100 species
~ 1000 reactions

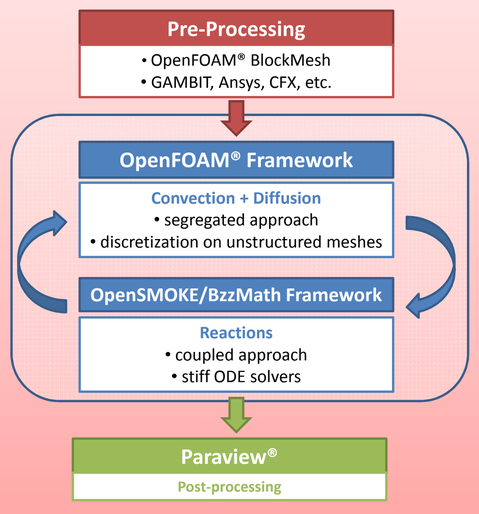
✓ fully coupled methods and fully segregated algorithms are unfeasible
✓ operator-splitting methods are an attractive solution

Complex CFD simulations



milions of computational cells

Methodology



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

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

where $\boldsymbol{\Psi}$ are the dependent 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. The integration is performed using the **Strang splitting** scheme. Reaction is separated from the transport process and the 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:

$$\frac{d\boldsymbol{\Psi}^a}{dt} = \mathbf{S}(\boldsymbol{\Psi}^a)$$

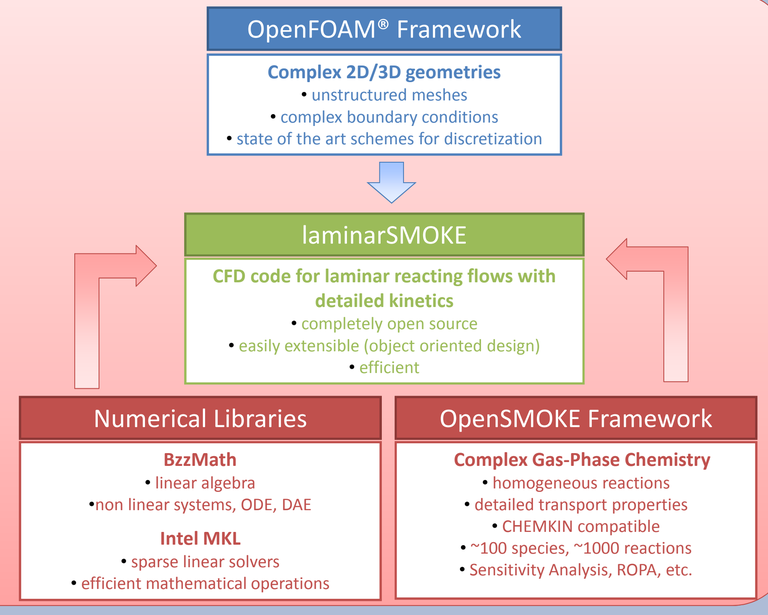
The initial condition $\boldsymbol{\Psi}^a(0)$ is equal to the final state $\boldsymbol{\Psi}$ from the previous step and the solution is indicated as $\boldsymbol{\Psi}^a(\Delta t/2)$.

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

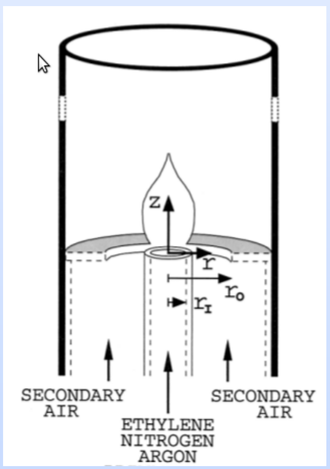
$$\frac{d\boldsymbol{\Psi}^b}{dt} = \mathbf{M}(\boldsymbol{\Psi}^b, t)$$

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

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.



Laminar coflow flame



Bennet, B.A., McEnally, C.S., Pfefferle, L.D., Smooke, M.D., Colket, M.B., *Computational and Experimental Study of Axisymmetric, Coflow Partially Premixed Ethylene/Air Flames*, Combustion and Flame (2001)

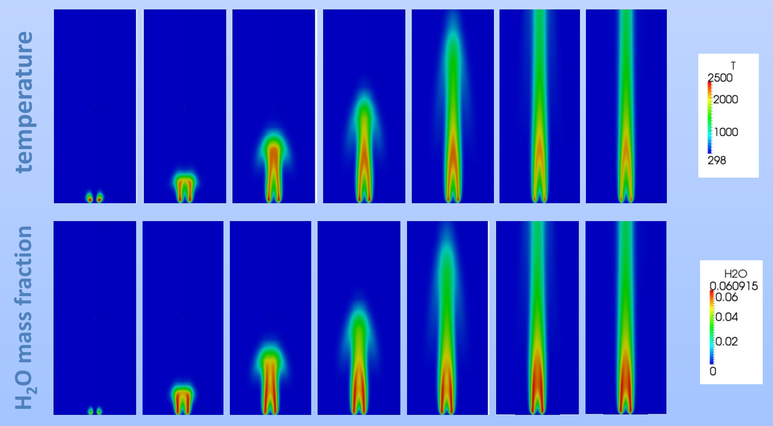
Fuel: $C_2H_4/N_2/Ar$ (30.14%, 68.42%, 1.42% mass)
Air: O_2/N_2 (23.2%, 76.8% mass)
Temperature = 298 K
Pressure = 1 atm
$\mathbf{V_{fuel}}$ = 12.52 cm/s
$\mathbf{V_{air}}$ = 32.60 cm/s

Geometry
Fuel nozzle internal radius = 5.55 mm
Combustion chamber internal radius = 55mm
Copper ring internal radius = 27.5 mm

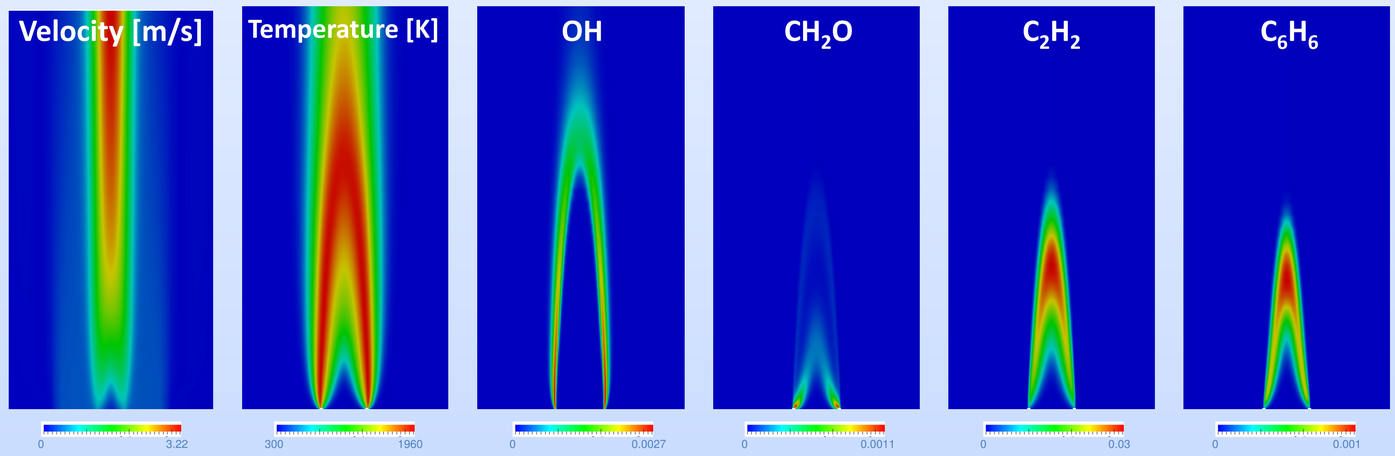
Experimental data
Measurements along the axis
T, C_2H_4, O_2, CO_2, CO, H_2O, H_2, CH_2O, C_6H_6, soot

Ignition

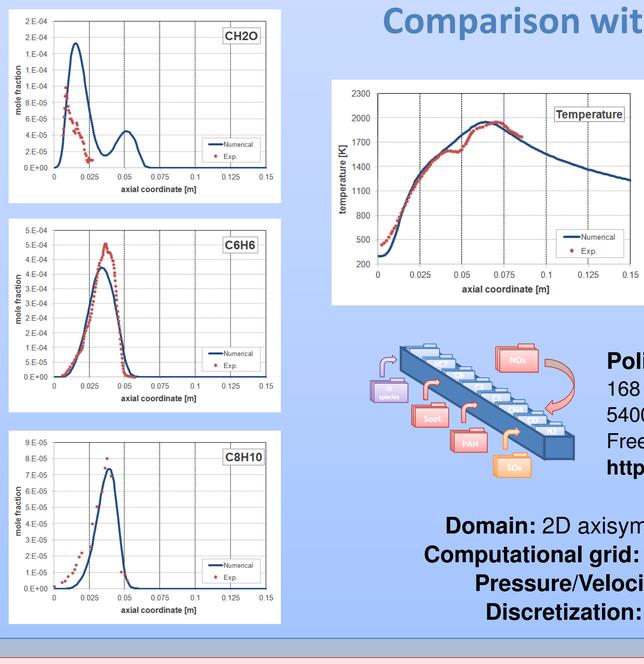
At *t=0* the initial composition is pure air at ambient temperature. A spark, located close to the fuel nozzle was applied in order to ignite the fuel mixture which is fed through the fuel nozzle. The duration of the spark is 0.20 s.



Results



Comparison with experimental data



PolimiC1C16HT kinetic scheme
168 species
5400 reactions
Freely available in CHEMKIN format at:
http://creckmodeling.chem.polimi.it/

Domain: 2D axisymmetric (55 x 200 mm)
Computational grid: ~5000 cells (structured)
Pressure/Velocity coupling: PISO
Discretization: first order upwind

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