Numerical modeling of laminar flames with detailed kinetics
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Motivation
The detailed numerical simulation of multidimensional laminar flames poses realistic chemical mechanisms, 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.

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:
\[
\frac{d\mathbf{y}}{dt} = \mathbf{S}(\mathbf{y})
\]

where \( \mathbf{y} \) are the dependent variables (mass fractions and enthalpies), \( \mathbf{S}(\mathbf{y}) \) is the rate of change of \( \mathbf{y} \) due to chemical reactions and \( \mathbf{M}(\mathbf{y}) \) the rate of change of \( \mathbf{y} \) due to transport processes. The integration is performed using the Strong 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 \( \Delta t \) through the solution of a ODE system:
\[
\frac{\mathbf{y}(t + \Delta t)}{\Delta t} = \mathbf{S}(\mathbf{y}(t))
\]

The initial condition \( \mathbf{y}(0) \) is equal to the final state \( \mathbf{y} \) from the previous step and the solution is indicated as \( \mathbf{y}(\Delta t) \).

Sub-step 2. The transport terms (convection and diffusion) are integrated over a time interval \( \Delta t \) by solving:
\[
\mathbf{y}(t + \Delta t) = \mathbf{y}(t) + \mathbf{M}(\mathbf{y}(t)) \Delta t
\]

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

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.

Results

Comparison with experimental data

Domain: 2D axisymmetric (55 x 200 mm)
Computational grid: 5400 cells
Fully available in CHEMKIN format at: http://creckmodeling.chem.polimi.it/

Velocity: [m/s] 0 0.001 0.002 0.003 0.004 0.005 0.006 0.007 0.008 0.009 0.01
Temperature: [K] 0 300 600 900 1200 1500 1800 2100 2400 2700 3000

References
[5] PolimiC1C16HT kinetic scheme
168 species, ~1000 reactions
Freely available in CHEMKIN format at: http://creckmodeling.chem.polimi.it

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“Cinica dettagliata di formazione di idrocarburi polinomiaci e nanoparticelle da processi di combustione”.

Pre-Processing
- OpenFOAM® BlockMesh
- GAMBIT, ANSYS, CFX, etc.

OpenFOAM® Framework
- General purpose software
- state of the art schemes for discretization
- Parallel processing

OpenSMOKE/BuzzMath Framework
- Large scale CFD
- Non-stiff systems

LaminarSMOKE
- CFD code for laminar reacting flows with detailed kinetics
- operatore-splitting schemes
- efficient mathematical operations

Paradigm®
- Pre-processing

Paradigm®
- Post-processing

OpenSMOKE Framework
- Complex 2D/3D geometries
- unstructured meshes
- conjugate heat transfer
- state of the art schemes for discretization
- completely open source

General reaction system
\[
\frac{d\mathbf{y}}{dt} = \mathbf{S}(\mathbf{y})
\]

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 \( 0.20 \text{ s} \).

Bennet B. A., et al., Computational and Experimental Study of Axisymmetric, Cold Partially Premixed Ethylene/ Air Flames, Combustion and Flame 2001

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