# laminarSMOKE: A computational framework for the modeling of laminar flows with detailed kinetic mechanisms

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## Motivation

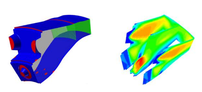
The detailed numerical simulation of **multidimensional laminar flames** flows with realistic chemical mechanisms is a challenging problem and places severe demands on computational resources. When **detailed kinetic mechanisms** are used, special attention has to be paid to the numerical algorithms, which must be accurate and efficient. The computational effort in terms of CPU time and memory requirements is considerable and in many cases prohibitive.

In this work we developed a numerical solver for OpenFOAM®, called **laminarSMOKE**, based on the **operator-splitting** technique, to simulate laminar flames in complex geometries with detailed kinetic schemes.

**Detailed kinetic schemes**


**~ 100 species**
**~ 1000 reactions**

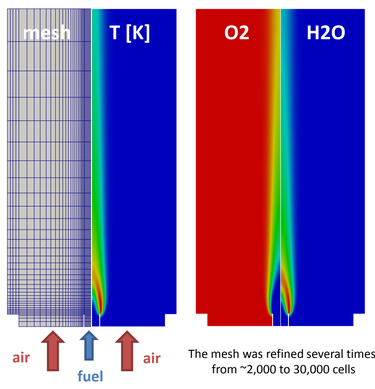
**Complex CFD simulations**



**millions of computational cells**

## Hydrogen flames

**V. V. Toro, A. V. Mokhov, H. B. Levinsky, M. D. Smooke,** *Proceedings of the Combustion Institute,* 30 (2005), 485-492



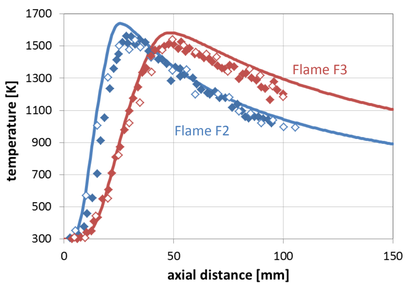

The mesh was refined several times, from ~2,000 to 30,000 cells

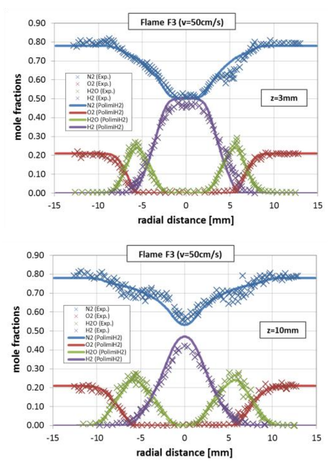
The coflow flames experimentally studied by Toro et al., were chosen as a first validation case. The fuel stream **(50% $H_2$ and 50% $N_2$ by volume)** is injected at ambient temperature through a circular nozzle (**i.d. 9 mm**), surrounded by an air-coflow annulus (**i.d. 95 mm**).

Two different average fuel exit velocities are considered: **27 cm/s (Flame F2)** and **50 cm/s (Flame F3)**.

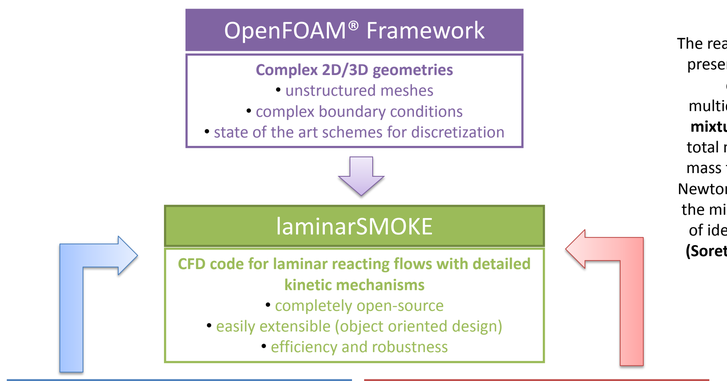
A **2D rectangular domain**, initially meshed with a structured grid, was considered. The fuel velocity profile was always assumed **parabolic**, while a flat velocity profile was imposed for the coflow stream.

Comparison between predictions and measurements along the center-line in terms of temperature. The agreement is quite satisfactory, especially for Flame F3.




## laminarSMOKE Framework




The code is specifically conceived for managing complex kinetic mechanisms and detailed transport properties in CHEMKIN format.

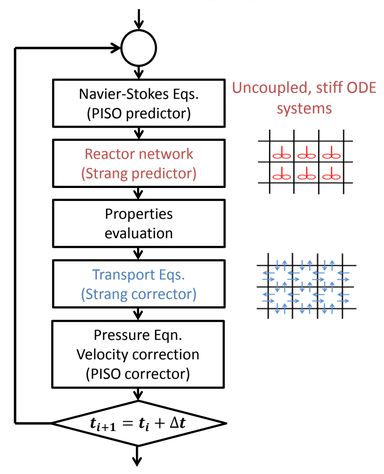
| Name | Language | Linear system solution | Code available | Web address |
|---|---|---|---|---|
| BzzMath6 | C++ | Direct | No | http://homes.chem.polimi.it/gbuzzi/index.htm |
| DVODE | FORTRAN | Direct | Yes | https://computation.llnl.gov/casc/odepack/odepack_home.html |
| CVODE | C | Direct/Iterative | Yes | https://computation.llnl.gov/casc/sundials/main.html |
| DLSODE | FORTRAN | Direct | Yes | https://computation.llnl.gov/casc/odepack/odepack_home.html |
| DLSODA | FORTRAN | Direct | Yes | https://computation.llnl.gov/casc/odepack/odepack_home.html |
| RADAU5 | FORTRAN | Direct | Yes | http://www.unige.ch/~hairer/software.html |
| LIMEX4 | FORTRAN | Direct | Yes | http://www.zib.de/en/numerik/software/codelib |
| MEBDF | FORTRAN | Direct | Yes | http://www2.imperial.ac.uk/~jcash/IVP_software |

The reactive, laminar flows under investigation in the present work are mathematically described by the conservation equations for continuous, multicomponent, compressible, thermally-perfect **mixtures of gases**. The conservation equations of total mass, mixture momentum, individual species mass fractions and mixture energy are solved for a Newtonian fluid in laminar conditions. The density of the mixture is calculated using the equation of state of ideal gases. Both **Fickian and thermal diffusion (Soret effect)** are taken into account for evaluating the diffusion velocities.

The first release of the code is expected in September 2012

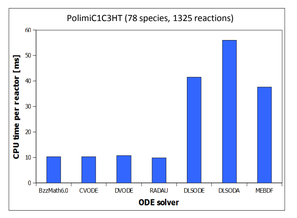
**www.opensmoke.polimi.it**

**Operator splitting-algorithm**




The numerical procedure is based on the **Strang splitting algorithm** (G. Strang, SIAM Journal of Numerical Analysis 5 (1968) 506-517). The mass fraction and enthalpy equations are integrated in two sub-steps. The first step involves only the reaction term, which is local and which is integrated using a stiff ODE solver. Convection and diffusion (second sub-step) are integrated using the implicit Euler method in the context of a fully segregated approach.

The core of the laminarSMOKE framework is the efficient solution of the large number of stiff ODE systems in the chemical step. Several stiff ODE solvers available on the web were tested and compared in terms of performances. Most of them showed a satisfactory robustness, also for large kinetic schemes. The best performances were obtained by the **BzzMath**, **CVODE** and **DVODE** solvers.



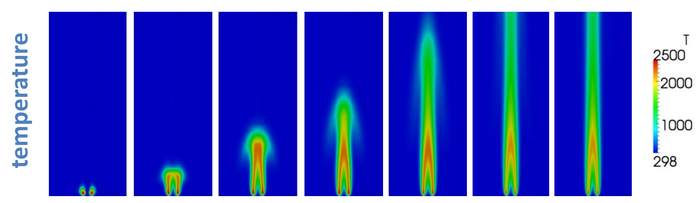

For each solver a C++ wrapper was created in order to have a object oriented style code

```
ODESystem_DVODE *odeSystemObject;
odeSystemObject = ODESystem_DVODE::GetInstance();

OpenSMOKE::OpenSMOKE_DVODE<ODESystem__DVODE>
                        ode(odeSystemObject);

ode.SetMaximumNumberOfSteps(100000);
ode.SetInitialValues(t0,Y0);
ode.Solve(tf);
ode.Solution(yF);
```

### 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*".

## Unsteady simulations




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.

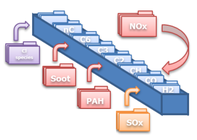
## Ethylene/Methane flames

**J.F. Roesler, M. Martinot, C.S. McEnally, L.D. Pfefferle, J.L. Delfau, C. Vovelle,** *Combustion and Flame,* 134 (2003) 249-260.

**Flame details**
**Fuel:** $CH_4/C_2H_4$
**Air:** $O_2/N_2$ (23.2%, 76.8% mass)
**Temperature:** 298 K
**Pressure:** 1 atm
**$V_{fuel}$:** 12.52 cm/s
**$V_{air}$:** 10.50 cm/s

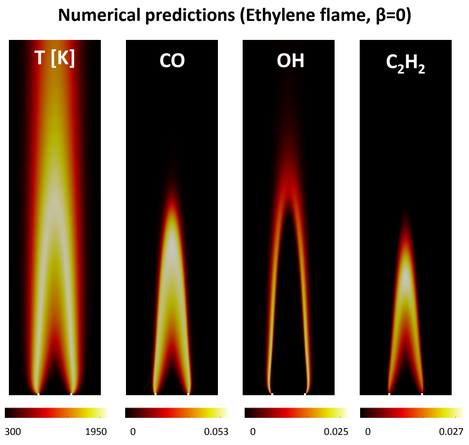
**Geometry**
**Fuel nozzle diameter:** 11.1 mm
**Chamber diameter:** 110 mm

**Computational details**
**Domain:** 2D axisymmetric (55 x 200 mm)
**Computational grid:** ~25,000 cells
**Discretization:** second order centered




**PolimiC1C16HT kinetic scheme**
168 species
5,400 reactions
Freely available in CHEMKIN format at:
**http://creckmodeling.chem.polimi.it/**

**Numerical predictions (Ethylene flame, β=0)**

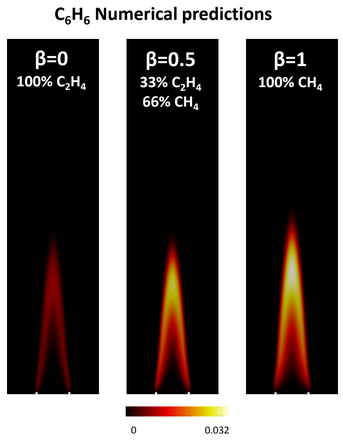


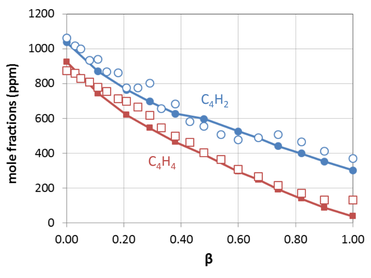

Roesler et al. experimentally studied a series of coflow flames, fed with a **mixture of $C_2H_4$, $CH_4$, and $N_2$** in different amounts.
The relative concentrations of $C_2H_4$ and $CH_4$ are identified by the **mixture parameter β**:

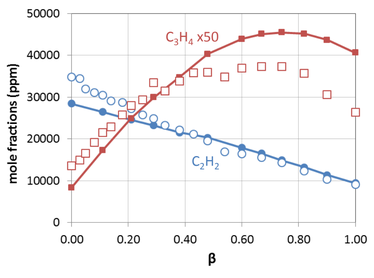
$$\beta = \frac{X_{CH4}}{X_{CH4} + 2X_{C2H4}}$$

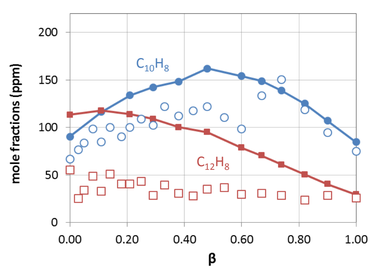
The maximum temperature and concentrations of species along the center-line were experimentally measured as a function of β. The plots reported below show the comparison between numerical values (lines) and experimental data (points) for several species.

**$C_6H_6$ Numerical predictions**



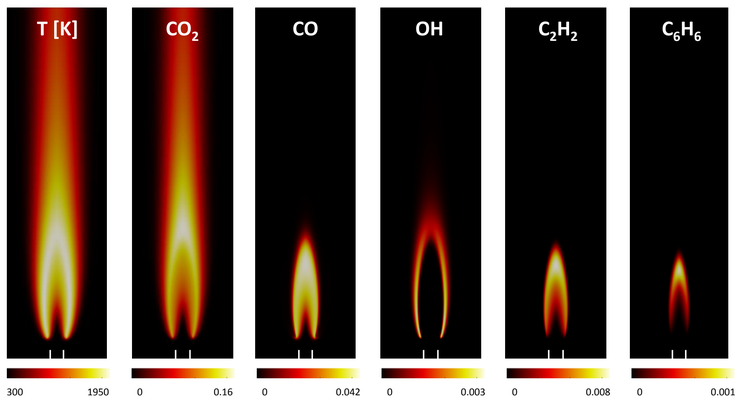




## Lifted flame

**R. H. Mohammed, M. A. Tanoff, M. D. Smooke, A. M. Shaffer,** *Proceedings of the Combustion Institute,* 27 (1998) 693-702.




**Flame details**
**Fuel:** $CH_4/N_2$ (51.5%, 48.5% mass)
**Air:** $O_2/N_2$ (23.2%, 76.8% mass)
**Temperature:** 298 K
**Pressure:** 1 atm
**$V_{fuel}$:** 35 cm/s
**$V_{air}$:** 35 cm/s

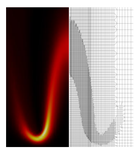
**Geometry**
**Fuel nozzle diameter:** 4 mm
**Coflow diameter:** 5 mm

**Computational details**
**Domain:** 2D axisymmetric (55 x 200 mm)
**Computational grid:** ~25,000 cells
**Discretization:** second order centered

**Kinetic schemes**
**GRI30:** 53 species, 325 reactions
**PolimiC1C16HTNOX:** 168 species, 5,400 reactions

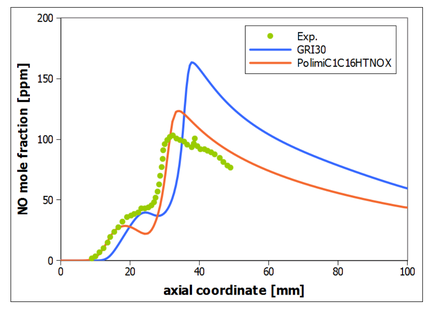
The maximum temperature along the center-line is 1930 K at 3.55 cm, in good agreement with computations performed by Mohammed et al. The peak temperature of 1950 K does not occur at the center line, but in the "wings" at a radius of 3.75 mm.

Numerical simulations predict a **flame lift-off of 2.6 mm**, which agrees with the experimental data of Mohammed et al., who measure a **flame lift-off of 2.2 mm**.

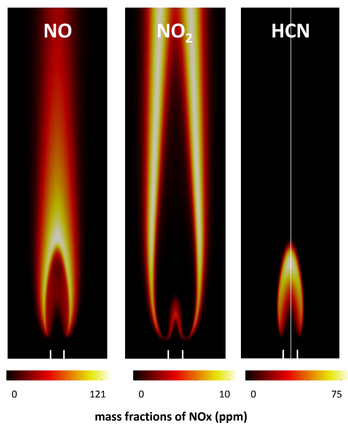


The flame-lift off was obtained by looking at the $HO_2$ mass fraction maps, reported above. In order to correctly capture the lift-off of the flame several local refinement of the mesh were performed.

**NOx predictions**




**M.D. Smooke, A. Ern, M.A. Tanoff, R.H. Mohammed, D.F. Marran, B. Long**
*Proceedings of the Combustion Institute,* 26 (1996) 2161-2170.

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