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

A. Cuoci, A. Frassoldati, T. Faravelli, E. Ranzi
Department of Chemistry, Materials and Chemical Engineering, Politecnico di Milano
Piazza Leonardo da Vinci 32, 20133, Milan, Italy

Motivation
The detailed numerical simulation of multidimensional/laminar flows with realistic chemical mechanisms is a challenging problem and places severe demands on computational resources. When detailed kinetic schemes 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 may be prohibitive.

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

Hydrogen flames


- Operator splitting algorithm
- Complex 2D simulations
- Detailed kinetic schemes

Unsteady simulations

Chemical Reaction Engineering and Chemical Kinetics, 41 (2016) 128-140

- Operator splitting algorithm
- Detailed kinetic schemes

Lifted flame


- Operator splitting algorithm
- Complex 2D/3D geometries
- Detailed kinetic schemes

Acknowledgements
Financial support for this activity was provided by the MIUR (Ministero dell’Istruzione dell’Universita e della Ricerca), under the PRIN 2004 framework: “Chemical mechanisms of homogeneous and heterogeneous processes at combustion”.

Unsteady simulations

- Operator splitting algorithm
- Detailed kinetic schemes

Lifted flame

- Operator splitting algorithm
- Complex 2D/3D geometries
- Detailed kinetic schemes

The peak temperature of 1950 K does not exceed 1930 K at 3.55 cm, in good agreement with the measured temperature of 1950 K.

The maximum temperature of 1950 K is injected at ambient conditions by the spark. The peak temperature of 1950 K does not exceed 1930 K at 3.55 cm, in good agreement with the measured temperature of 1950 K.

The plots of concentration of species along the center line were experimentally measured. The plots reported below show the comparison between measured and calculated concentrations of species along the center line.

The maximum temperature along the center line is 1930 K at 3.55 cm, in good agreement with the measured temperature of 1950 K.

The best performances were obtained by the FORTRAN code SMOKE®. The BzzMath® code was created in order to have a hybrid unsteady code.