Iran First International Combustion School (ICS2019)
Tehran, 24-26 August 2019

Combustion modeling: Training Sessions

3. Numerical modeling of 1D flames: Laminar flame speed and counterflow diffusion flames

Alberto Cuoci

The OpenSMOKE++ Suite

- The **OpenSMOKE++ Suite** (developed by the CRECK Modeling Group at Politecnico di Milano) is a collection of standard solvers for simulating reacting systems with detailed kinetic mechanisms, with hundreds of species and thousands of reactions.

- The solvers currently available move from ideal reactors (batch reactors, continuously stirred tank reactors, plug flow reactors, …) to laminar premixed and diffusive laminar flames. Heterogeneous catalytic reactions are also accounted for.

- The OpenSMOKE++ Suite can be freely downloaded from the following website address, after registration from an Academic email address: https://www.opensmokepp.polimi.it/

- Details are available in the following paper:

Cuoci, A., Frassoldati, A., Faravelli, T., Ranzi E., *OpenSMOKE++: An object-oriented framework for the numerical modeling of reactive systems with detailed kinetic mechanisms*, Computer Physics Communications, 192, p. 237-264 (2015), DOI: 10.1016/j.cpc.2015.02.014

Organization of ICS2019 Training Session Material

TrainingSessions

- TS1
- TS2
- Docs
- KineticMechanisms

`TS1, TS2, …`
Folders containing the input files needed to carry out the tasks corresponding to the training sessions 1, 2, etc

`Docs`
OpenSMOKE++ User's Guide and additional documentation files

`KineticMechanisms`
Collection of several detailed kinetic mechanisms in CHEMKIN format (thermodynamics, transport and kinetic files) adopted for running the simulations

OpenSMOKE++ User's Guide & Tutorials

- The OpenSMOKE++ User's Guide is available in the Docs folder
- All the available options for each solver are reported there, together details about the installation process
- Additional examples and tutorials are available at the following web address: https://github.com/acuoci/OpenSMOKEppTutorials

Outline

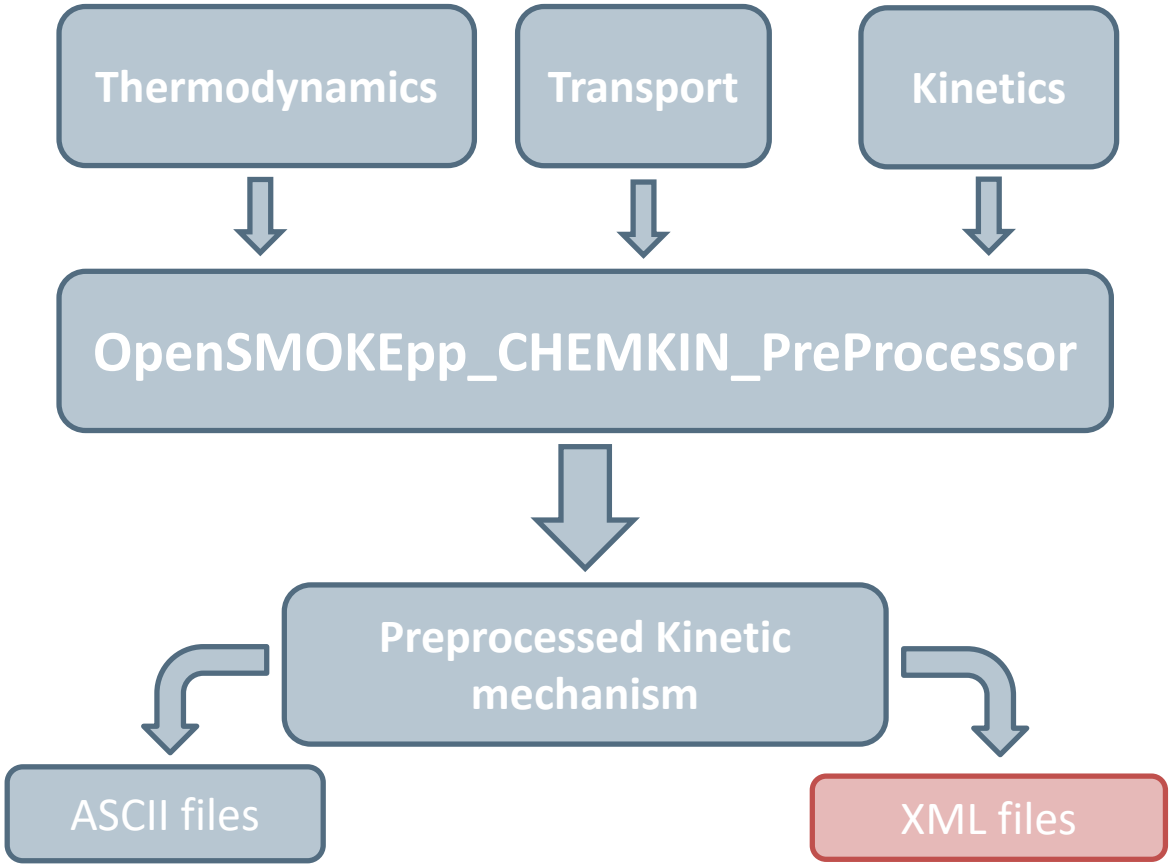
0. **Pre-processing of a kinetic mechanism**

1. **Laminar flame speed of a syngas (H2/CO) mixture in air**

2. **Parametric analysis of laminar flame speed of a syngas (H2/CO) mixture in air**

3. **Exercise: laminar flame speed of a gasoline surrogate**
   a) toluene
   b) n-heptane/iso-octane

Task 0: pre-processing kinetic mechanisms



Objective: get familiar with the pre-processing operations and analysis of pre-processed results

Task: preprocess a complete kinetic mechanism (together with thermodynamics and transport properties)

We will use the `POLIMI_H2CO_1412.CKI` kinetic mechanism (14 species, 33 reactions), a detailed mechanism for the combustion of H2 and CO mixtures

Task 0: pre-processing kinetic mechanisms

1. Preparation of input data

Go to the `Task0` folder, containing the `input.dic`. This file contains instructions for pre-processing the complete kinetic mechanism

```
Dictionary CHEMKIN_PreProcessor
{
        @Thermodynamics
        ../../KineticMechanisms/POLIMI_1412/Thermodynamics/POLIMI_TOT_NOX_1412.CKT;
        @Transport
        ../../KineticMechanisms/POLIMI_1412/Transport/POLIMI_TOT_NOX_1412.TRC;
        @Kinetics
        ../../KineticMechanisms/POLIMI_1412/Kinetics/POLIMI_H2CO_1412.CKI;
        @Output
        kinetics-POLIMI_H2CO_1412;
}
```

`@Transport`
path to the CHEMKIN file containing the transport data to be pre-processed

`@Kinetics`
path to the CHEMKIN file containing the kinetic mechanism to be pre-processed

Task 0: pre-processing kinetic mechanisms

2. Run the kinetic preprocessor

3. Analyze the pre-processing results

If everything was done properly, the `kinetics-POLIMI_H2CO_1412` output folder will be created, containing the following files (in addition to the usual files associated to thermodynamics):

`Kinetics_Summary.out`
This file simply contains the kinetic mechanism written in a more readable format

`kinetics.xml`
`reaction_names.xml`
these are the only file needed by OpenSMOKE++ Suite solvers. They contain the pre-processed thermodynamic (and transport) data together with the whole reaction mechanism in XML format

Laminar Flame Speed: preparation of input files (I)

1. Preparing the input for jet laminar flame speed calculations

The `Task1` folder contains the input files for calculating the laminar flame speed of a mixture with given composition, temperature and pressure. The input file is split in several Dictionaries.

```
Dictionary PremixedLaminarFlame1D
{
        @Type                   FlameSpeed;
        @KineticsFolder         ../Task0/kinetics-POLIMI_H2CO_1412;
        @InletStream            inlet-stream;
        @OutletStream           outlet-stream;
        @InletVelocity          50 cm/s;
        @Grid                   grid;
        @Output                 Output;
        @UseDaeSolver           true;
}
```

Main Dictionary for defining the main parameters of the flame to be simulated

Laminar Flame Speed: preparation of input files (II)

```
Dictionary inlet-stream
{
    @EquivalenceRatio    1;
    @FuelMoles           H2 0.40 CO 0.30 N2 0.3;
    @OxidizerMoles       O2 0.21 N2 0.79;
    @Temperature         300 K;
    @Pressure            1 atm;
}

Dictionary outlet-stream
{
    @Moles       H2O 0.15 CO2 0.15 N2  0.70;
    @Temperature 2300 K;
    @Pressure    1 atm;
}
```

Definition of the mixture

This is only a first guess

Laminar Flame Speed: preparation of input files (II)

```
Dictionary grid
{
        @Length                     4 cm;
        @InitialPoints              12;
        @Type                       database;

        @MaxPoints                  500;
        @MaxAdaptivePoints          15;
        @GradientCoefficient        0.03;
        @CurvatureCoefficient       0.5;
}
```

Definition of the initial computational grid

Definition of the adaptive grid algorithm

Laminar Flame Speed: running the code

2. Run the laminar flame speed calculations

Always from the same `Task1` folder, we can now run the `OpenSMOKEpp_PremixedLaminarFlame1D` solver.

Run the `Run.bat` file by double-clicking on it or, from the Command Prompt, type:

```
"%OPENSMOKEPP_EXE_FOLDER%\OpenSMOKEpp_PremixedLaminarFlame1D.exe" --
input input.dic
```

3. Analysis of output

The spatial profiles of velocity, temperature and compositions are available in the Temperature and composition at the exit of each simulated condition are available in the `Solution.final.out` file. The laminar flame speed velocity is defined as the velocity of the mixture at the inlet boundary

Parametric analysis

Usually, the laminar flame speed is evaluated at several equivalence ratios. The calculations can be carried out automatically in a user defined range of equivalence ratio. The `Task2` folder contains an example of this parametric analysis.

```
Dictionary inlet-stream
{
        @EquivalenceRatio       1 1.05 1.10 1.20 1.30
                                0.95 0.90 0.80 0.70;

        @FuelMoles              H2      0.70 N2 0.30;
        @OxidizerMoles          O2      0.21 N2 0.79;

        @Temperature            300 K;
        @Pressure               1 atm;
}
```

In most cases it is convenient (for numerical reasons only) to start from simulation of flame at stoichiometric conditions.

Task 3: Suggested exercise

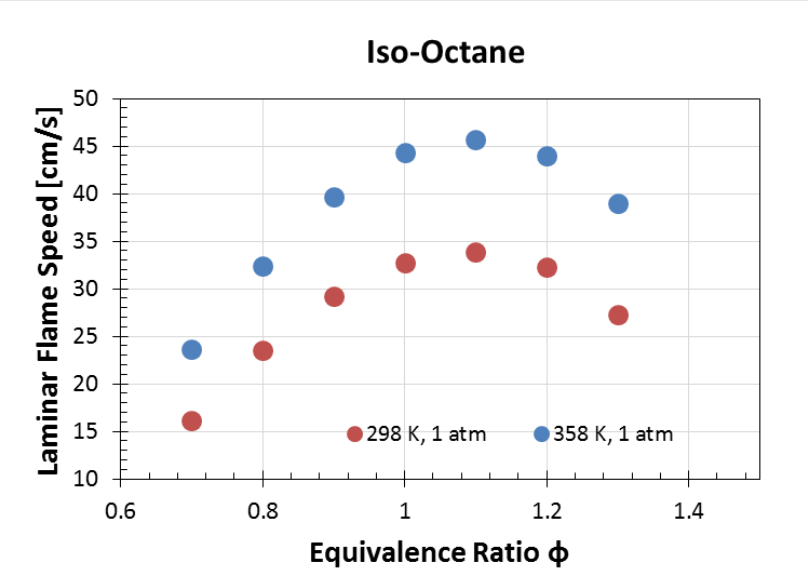
We propose to calculate the laminar flame speeds for n-heptane, iso-octane, toluene and a surrogate mixture of them (i.e. a gasoline) and compare the numerical results with the experimental data of **Sileghem et al. (2013)** reported in the following paper (see also next slides)

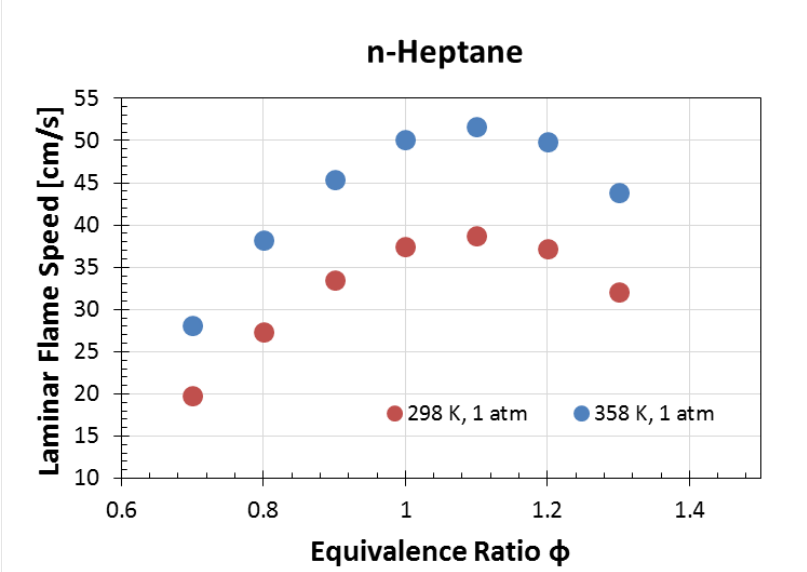
> **Sileghem et al.,** *Laminar burning velocity of gasoline and the gasoline surrogate components iso-octane, n-heptane and toluene*, Fuel, 112 (2013), p. 355-365

A proper kinetic mechanism must be adopted. We suggest to use the POLIMI_PRF_PAH_LT_1412 kinetic mechanism. Such a mechanism is quite large and thus the simulations will be quite long.

Experimental data (I)

Laminar burning velocities have been measured using the heat flux method on a flat flame adiabatic burner. Measurements were done for iso-octane, n-heptane, toluene, a toluene reference fuel (i.e., a mixture of iso-octane, n-heptane and toluene) and a commercial gasoline. Measurements were done for an equivalence ratio from 0.7 to 1.3 and for a range of temperatures between 298 K and 358 K.





Sileghem et al., *Laminar burning velocity of gasoline and the gasoline surrogate components iso-octane, n-heptane and toluene*, Fuel, 112 (2013), p. 355-365

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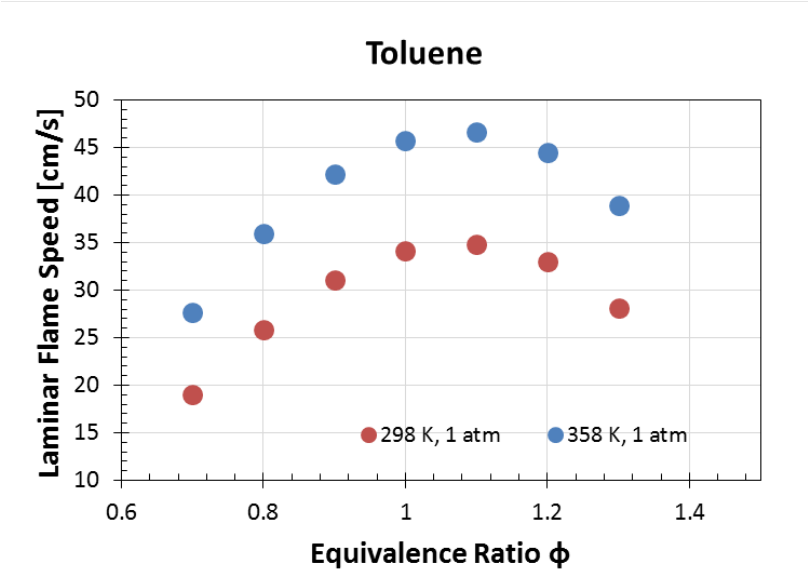
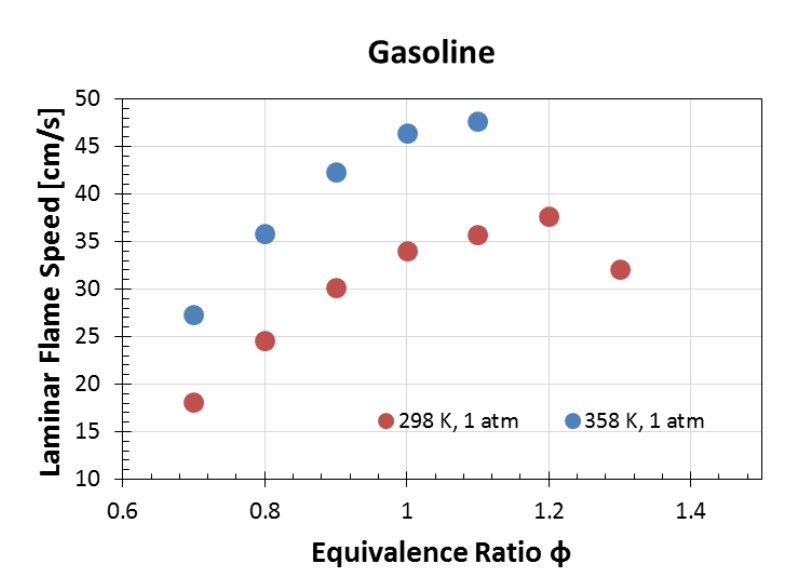
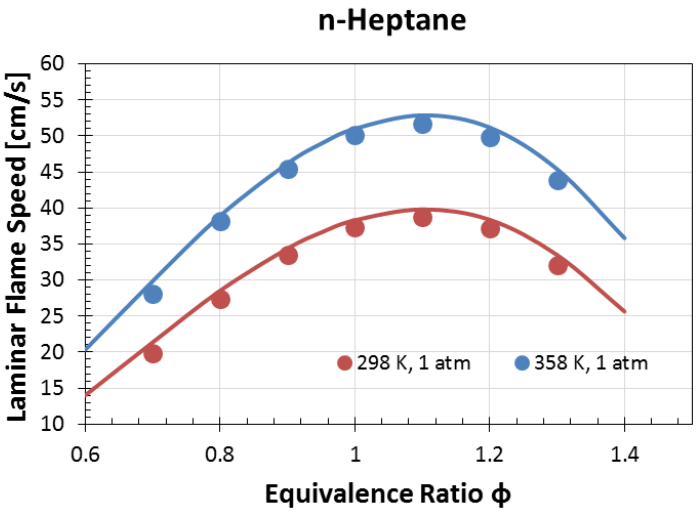
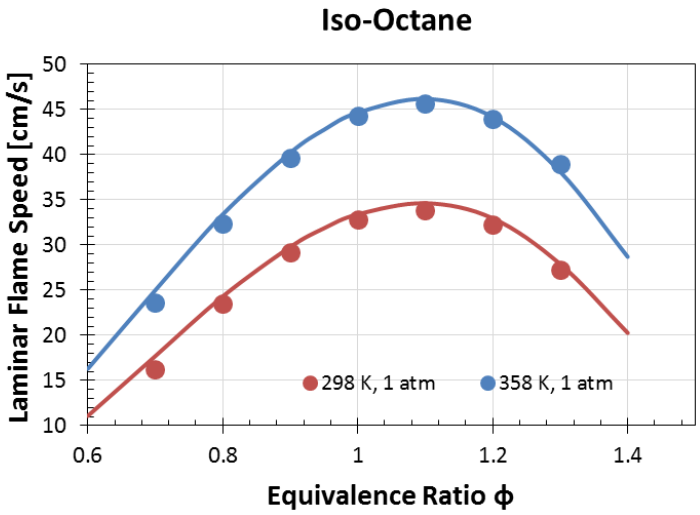


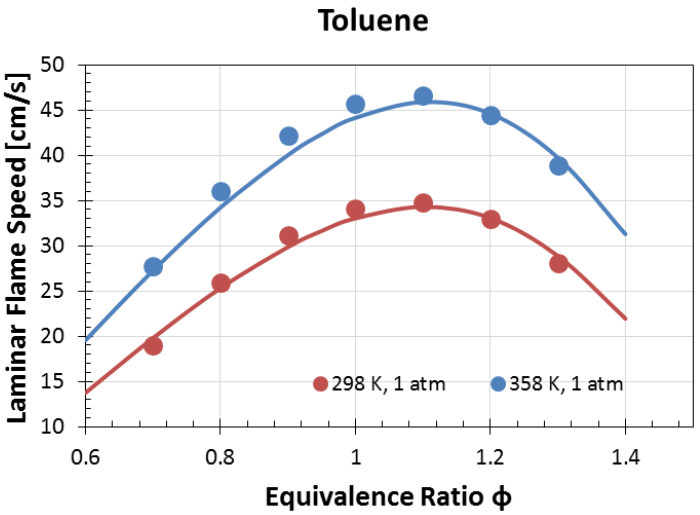


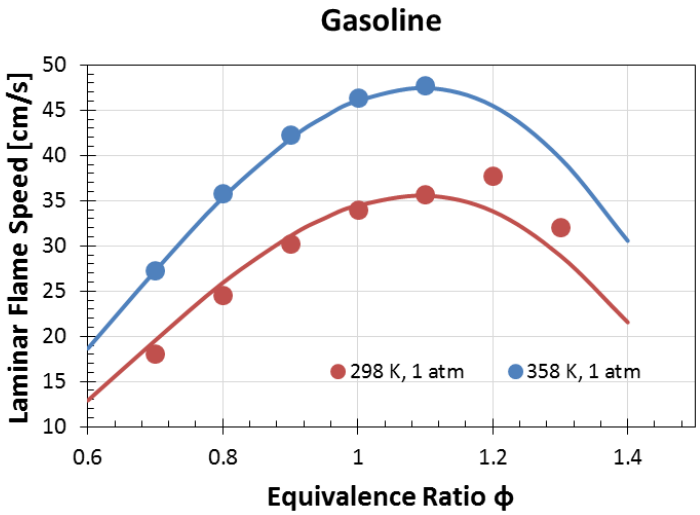
Sileghem et al., *Laminar burning velocity of gasoline and the gasoline surrogate components iso-octane, n-heptane and toluene*, Fuel, 112 (2013), p. 355-365

Comparison with experimental data









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OpenSMOKE++ Development

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