

libOpenSMOKE

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1 libOpenSMOKE

libOpenSMOKE is a set of additional libraries and solvers for OpenFOAM-1.7, specifically conceived to manage reacting flows with complex chemistry. In particular, the current 0.1 version implements the following steady-state and unsteady solvers for turbulent flame simulations:

rhoSimpleFoamFlamelets: a steady-state solver (based on the **rhoSimpleFoam** solver) for turbulent non premixed flames using the steady-state, laminar flamelet approach to manage interactions between chemistry and turbulence; look-up tables are generated using specific applications (see in the following), whose binaries are freely distributed with this library

rhoPisoFoamFlamelets: the unsteady version (based on the **rhoPisoFoam** solver) of **rhoSimpleFoamFlamelets** solver. Currently, the **rhoPisoFoamFlamelets** solver is under testing and validation procedure and will be available in the next releases.

rhoSimpleFoamPostProcessorSoot2E: a kinetic post-processor for evaluating formation of soot in steady-state, turbulent flames, based on the Method of Moments (soot particle number density and soot volume fraction are transported)

rhoSimpleFoamPostProcessorSootQMOM: a kinetic post-processor for evaluating formation of soot in steady-state, turbulent flames, based on the Quadrature Method of Moments (QMOM). Currently, the **rhoSimpleFoamPostProcessorSootQMOM** solver is under testing and validation procedure and will be available in the next releases.

References

If you use libOpenSMOKE library in your publications, please cite the following papers:

A. Cuoci, A. Frassoldati, T. Faravelli, E. Ranzi, “*Formation of soot and nitrogen oxides in unsteady counter flow diffusion flames*”, Combustion and Flame 156 (10), pp. 2010-2022 (2009)

A. Cuoci, A. Frassoldati, T. Faravelli, E. Ranzi, “*Kinetic modeling of soot formation in turbulent non premixed flames*”, Environmental Engineering Science, 25 (10), pp. 1407-1422 (2008)

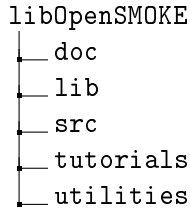


Figure 1.1: libOpenSMOKE library structure

1.1 Library description

The libOpenSMOKE library is organized in several folders, containing source code, utilities, documentation, examples, etc., which are briefly described in the following (see Figure 1.1):

- doc:** this folder contains the documentation for compiling and using the libOpenSMOKE library
- lib:** libOpenSMOKE compiled libraries are stored in this folder
- src:** source code to be compiled in OpenFOAM-1.7 can be found in this folder
- tutorials:** this folder contains several tutorials and examples about the use of libOpenSMOKE library and solvers
- utilities:** this folder contains several utilities to generate laminar, steady-state flamelets and look-up tables to be used in conjunction with libOpenSMOKE solvers

In the following subsections the content of each folder is described in details.

1.1.1 Source code

The core of the library is the **src** folder, containing the code to be compiled and linked with OpenFOAM-1.7. The source files are organized as reported in Figure 1.2.

The source files are available in two main folders: **applications** folder contains the code for the libOpenSMOKE solvers; the **libraries** folder contains the code for the following libOpenSMOKE sub-libraries:

- **common:** this sub-library contains some utilities and classes which can be called by the others sub-libraries (i.e. mathematical functions, probability distribution functions, etc.)
- **flamelets:** classes to manage steady state, non adiabatic flamelet libraries, for simulation of non-premixed, turbulent flames

```

src
├── applications
│   ├── rhoPisoFoamFlamelets
│   ├── rhoSimpleFoamFlamelets
│   ├── rhoSimpleFoamPostProcessorSoot2E
│   └── rhoSimpleFoamPostProcessorSootQMOM
└── libraries
    ├── common
    ├── flamelets
    ├── pdfThermo
    ├── qmom
    └── twoequations

```

Figure 1.2: src folder content

- **twoequations**: classes used to calculate soot formation in turbulent flames using the method of moments (2E Model)
- **qmom**: classes used to calculate soot formation in turbulent flames using the method of moments with the QMOM (Quadrature Method of Moments)
- **pdfThermo**: new thermodynamics to manage steady state, non adiabatic flamelet libraries directly in OpenFOAM

1.1.2 Utilities

This folder contains three main utilities needed by libOpenSMOKE library to perform numerical simulations of turbulent, non-premixed flames:

- **OpenSMOKE_CHEMKINInterpreter.sh**: utility to pre-process CHEMKIN mechanisms
- **OpenSMOKE_SteadyStateFlamelets.sh**: utility to generate flamelet profiles using detailed kinetics
- **OpenSMOKE_LookUpTable.sh**: utility to generate look-up tables to be used in libOpenSMOKE

In addition this folder contains some detailed kinetic mechanisms for hydrocarbon combustion and pyrolysis from CRECK (Chemical Reaction Engineering and Chemical Kinetics) Group at Politecnico di Milano. Both the CHEMKIN format and the pre-processed versions of each kinetic scheme are available.

1.1.3 Tutorials

This folder contains several tutorials about the use of libOpenSMOKE library:

- **Sandia_HE0**: this tutorial shows the application of non-adiabatic, laminar flamelet model to the Sandia HE0 Flame [2, 3, 6]
- **Sandia_COH2N2**: this tutorial shows the application of non-adiabatic, laminar flamelet model to the Sandia COH2N2 Flame [5, 4]
- **KentHonnery**: this tutorial shows the application of non-adiabatic, laminar flamelet model to the turbulent jet flame experimentally investigated by Kent and Honnery [17]
- **KentHonneryPostProcessing**: in this tutorial the KentHonnery case (see above) is post processed to estimate soot formation
- **LookUpTable_Assembling**: in this tutorial the generation of a non adiabatic look-up table is described

1.2 Compilation and Installation

1.2.1 Prerequisites

In order to compile the libOpenSMOKE library, the GSL (GNU Scientific Library) is required. This library can be freely downloaded at the following web address:

www.gnu.org/software/gsl/

1.2.2 Sub-libraries compilation and installation

In the following the detailed procedure to compile and install the libOpenSMOKE sub-libraries is reported.

1. Copy the libOpenSMOKE folder in your OpenFOAM folder:

```
cp -r libOpenSMOKE $FOAM_INST_DIR
```
2. Update the path to GSL library in `src/libraries/qmom/Make/options` and `src/libraries/pdfThermo/Make/options` files using the correct path on your machine
3. Clean the library using the Allwclean script in libOpenSMOKE/src/libraries

```
cd $FOAM_INST_DIR/libOpenSMOKE/src/libraries  
./Allwclean
```

4. Compile the library using the Allwmake script in libOpenSMOKE/src/libraries
cd \$FOAM_INST_DIR/libOpenSMOKE/src/libraries
./Allwmake

1.2.3 Solvers compilation and installation

In the following the detailed procedure to compile and install the libOpenSMOKE solvers is reported.

1. For each solver, update the path reported in the Make/files according to your preferences
2. For each solve, update the path to GSL library in Make/options
3. Clean the solvers using the Allwclean script in libOpenSMOKE/src/applications
cd \$FOAM_INST_DIR/libOpenSMOKE/src/applications
./Allwclean
4. Compile the solvers using the Allwmake script in libOpenSMOKE/src/applications
cd \$FOAM_INST_DIR/libOpenSMOKE/src/applications
./Allwmake

1.3 Kinetic schemes pre-processing

The libOpenSMOKE library requires detailed kinetic schemes, thermodynamic and transport properties in CHEMKIN format. However, to be effectively used, a CHEMKIN mechanism must be pre-processed. The OpenSMOKE_CHEMKINInterpreter.sh utility (available in utilities/exe folder) is used for this purpose. Several kinetic mechanisms, both in CHEMKIN format and already pre-processed can be found in the utilities/kinetics folder.

The OpenSMOKE_CHEMKINInterpreter.sh can be executed using the following command:

```
OpenSMOKE_CHEMKINInterpreter.sh -kinetics "KineticScheme.kin" -thermo  
"Thermodynamics.tdc" -transport "Transport.tra" -output "OutputFolder"
```

The kinetic scheme, thermodynamics and transport properties files are provided through the -kinetics, -thermo and -transport options respectively. In the output folder two binary files, idealgas.bin and reactions.bin, are generated, containing the interpreted kinetic scheme, together with thermodynamic and transport properties. Moreover, additional files containing additional information are available (these files are not strictly necessary and can be deleted).

Several kinetic schemes, together with transport properties and thermodynamic data, are distributed together with the `libOpenSMOKE` library. They were developed by CRECK (Chemical Reaction Engineering and Chemical Kinetics) Group at Politecnico di Milano and can be also freely downloaded at the following web address:

<http://creckmodeling.chem.polimi.it/>

1.4 Look-Up Table construction

The `rhoSimpleFoamFlamelets` solver requires the calculation of a look-up table, in which temperature, mass fractions and physical properties (density, thermal conductivity, viscosity, etc.) are stored as a function of 3 independent variables: mixture fraction, scalar dissipation rate and enthalpy defect. The `rhoSimpleFoamFlamelets` solver applies a suitable set of PDFs (Probability Distribution Functions) to the flamelet profiles stored in the look-up table, according to the local values (i.e. in each computational cell) of independent variables:

$$\tilde{\psi} = \int_{-\infty}^{\infty} \int_0^{\infty} \int_0^1 \psi(Z, \chi_{st}, \phi_H) P(Z) P(\chi_{st}) P(\phi_H) dZ \cdot d\chi_{st} \cdot d\phi_H \quad (1.1)$$

Usually, a β -PDF or a clipped-Gaussian PDF is used for Z (mixture fraction space), a log-normal distribution for χ_{st} (scalar dissipation rate space) and a delta-Dirac function for ϕ_H (enthalpy defect space).

In order to save computational time during the CFD calculation, the integration with respect the mixture fraction is pre-calculated and stored in the look-up table. This means that the real look-up table which is managed by the `rhoSimpleFoamFlamelets` is defined on 4 independent variables: mixture fraction Z , scalar dissipation rate χ_{st} , enthalpy defect ϕ_H and variance of mixture fraction $\widetilde{Z''^2}$. This last variable is needed to perform the integration in the mixture fraction space, since both the β -PDF and the clipped-Gaussian PDF require the knowledge of the mixture fraction variance to be completely defined. Therefore, only the integration in the scalar dissipation rate space is performed by the `rhoSimpleFoamFlamelets` solver.

The construction of a look-up table consists of three main steps:

1. generation of flamelets profiles at several scalar dissipation rates (from equilibrium conditions to extinction) and several enthalpy defects;
2. application of β -PDF (or clipped-Gaussian PDF) in the mixture fraction space to flamelets profiles previously calculated;
3. assembling of the whole look-up table.

The first two steps reported above are managed by two different applications, respectively called `OpenSMOKE_SteadyStateFlamelets.sh` and `OpenSMOKE_LookUpTable.sh`, which must be strictly applied in sequence. In the following a brief description of each tool is reported.

```

// ----- //
// Flamelet //
// ----- //
#Fuel CH4
#Oxidizer O2
#Inert N2
#Points 80
#Pressure 1 atm
#FuelTemperature 333. K
#FuelMoleFractions CH4 0.95 C2H6 0.025 CO2 0.005 N2 0.02
#OxidizerTemperature 292. K
#OxidizerMoleFractions O2 0.21 N2 0.79
#FlameTemperature 2200. K
#FlamePosition 0.90
#OutputSpecies ALL
#ScalarDissipationRates 1.e-6 1.e-4 1e-2 1. 5. 10. 20. 30. 40. 45. Hz
#EnthalpyDefect -100.0 kJ/kg
#MinimumTemperature 292 K
#RelativeTolerance 1.e5
#END

```

Figure 1.3: Example of Data.inp file for OpenSMOKE_SteadyStateFlamelets.sh

1.4.1 OpenSMOKE_SteadyStateFlamelets

The OpenSMOKE_SteadyStateFlamelets.sh allows the user to generate a set of steady-state, laminar flamelets with different scalar dissipation rates at a fixed value of enthalpy defect. If additional enthalpy defects are needed, the OpenSMOKE_SteadyStateFlamelets.sh utility can be reused specifying the required enthalpy defect value.

The OpenSMOKE_SteadyStateFlamelets.sh requires a detailed kinetic scheme and two input files (which will be called in the following as Data.inp and Operations.inp). The Data.inp file contains the flamelet definition, while the Operations.inp file additional details about the numerical procedure to obtain the flamelet solution. A typical Data.inp file is reported in Figure 1.3.

Comments are introduced by a // and can be inserted in every point. Key words always begin with the # symbol. In Table 1.1, an explanation of each row is reported.

The Operations.inp file is used to suggest the grid refining operations to be performed to obtain accurate flamelets solutions. An example of Operations.inp file is reported in Figure 1.4.

The command SOLVE 1e5 means that the flamelet profile must be solved on the current grid using a transient integration method, for 1.e5 seconds (to reach steady state conditions). REFINELEANSIDE 0.65 command requires grid refining on the lean side of the flamelet, in the region where temperature are at least 0.65 times the peak temperature. NEWPOINTS TEMPERATURE D command requires grid refining on the whole mixture frac-

Option	Description
#Fuel	Name of fuel species
#Oxidizer	Name of oxidizer species
#Inert	Name of inert species
#Points	Number of initial grid points
#Pressure	Pressure
#FuelTemperature	Temperature of fuel inlet stream
#OxidizerTemperature	Temperature of oxidizer inlet stream
#FuelMoleFractions	Composition (in mole fractions) of fuel inlet stream. Alternatively the #FuelMassFractions keyword can be used.
#OxidizerMoleFractions	Composition (in mole fractions) of oxidizer inlet stream. Alternatively the #FuelMassFractions keyword can be used.
#ScalarDissipationRates	List of scalar dissipation rates to be calculated
#EnthalpyDefect	Enthalpy defect value (adiabatic conditions corresponds to a value of 0 kJ/kg)
#FlameTemperature	First guess value of peak temperature
#FlamePosition	First guess value of peak temperature position (in the mixture fraction space)
#OutputSpecies	List of species to be written in the output files (ALL means that every species in the kinetic mechanisms is considered)
#MinimumTemperature	Minimum temperature value for non adiabatic calculations
#RelativeTolerance	Relative tolerance for ODE system solution. The value 1.e5 is internally multiplied by the machine epsilon

Table 1.1: Options in Data.inp file for OpenSMOKE_SteadyStateFlamelets

```

SOLVE 1e5
REFINELEANSIDE 0.65 SOLVE 1e5
REFINELEANSIDE 0.80 SOLVE 1e5
REFINELEANSIDE 0.90 SOLVE 1e5
REFINELEANSIDE 0.90 SOLVE 1e5
CYCLE 4
NEWPOINTS TEMPERATURE D SOLVE 1e5
NEWPOINTS TEMPERATURE G SOLVE 1e5
ENDCYCLE
END

```

Figure 1.4: Example of `Operations.inp` file for `OpenSMOKE_SteadyStateFlamelets.sh`

tion space in regions where the temperature gradient is not well described. `NEWPOINTS TEMPERATURE G` command requires grid refining on the whole mixture fraction space in regions where the temperature curvature is not well described. Loops can be specified through the `CYCLE N ... ENDCYCLE` commands. The operations (...) between `CYCLE` and `ENDCYCLE` keywords must be repeated N times.

The `OpenSMOKE_SteadyStateFlamelets` utility can be executed by specifying the detailed kinetic scheme folder and the input files, according to the following syntax:

```

OpenSMOKE_SteadyStateFlamelets.sh --kinetics "KineticScheme" --input "Data.inp"
--schedule "Operations.inp"

```

Output files are stored in a folder whose name is `Flamelet_XXX`, where `XXX` is the name of the kinetic scheme adopted for calculations. Flamelet profiles are available in the `Steady` sub-folder, with names like `Final_YYY_Hz.out`, where `YYY` is the scalar dissipation rate value.

1.4.2 OpenSMOKE_LookUpTable

Flamelets profiles calculated in the previous step must be processed by applying a suitable PDF in the mixture fraction space to be used in CFD calculations. This operation can be performed using the `OpenSMOKE_LookUpTable.sh` utility, which requires a detailed kinetic scheme (of course the same used for generation of flamelet profiles) and an input file (which will be called `Data.inp` in the following), describing some options concerning PDF integration. Suppose that a set of 3 flamelets was generated using the `OpenSMOKE_SteadyStateFlamelets.sh` utility and we want to apply a β -PDF using the `OpenSMOKE_LookUpTable.sh` utility. The corresponding `Data.inp` file is reported in Figure 1.5. The meaning of each option is reported in Table 1.2.

The `OpenSMOKE_LookUpTable.sh` utility can be executed from the command line by specifying the detailed kinetic scheme folder and the input file, according to the following syntax:

```

// _____ //
// LookUp Table //
// _____ //
#Pdf BETA
#ListOfFlamelets Final_1e-005_Hz.out Final_0.0001_Hz.out Final_0.001_Hz.out
#FlameletLibrary PDF+200 fla
#LookUpTable PDF+200 lib
#LookUpTableOpenFOAM PDF+200-Lib
#NumberOfVariances 32
#StretchingFactor 1.17
#END

```

Figure 1.5: Example of Data.inp file for OpenSMOKE_LookUpTable.sh

Option	Description
#Pdf	Kind of probability distribution function to be applied in the mixture fraction space. BETA and GAUSSIAN options are available
#ListOfFlamelets	List of flamelet profiles to be post-processed. These profiles were obtained using the OpenSMOKE_SteadyStateFlamelets utility
#FlameletLibrary	Flamelets profiles can be collected in a single file with (with fla extension), which can be imported in FLUENT commercial CFD code
#LookUpTable	The look-up table can be generated in a format (with lib extension) which can be imported in FLUENT commercial code
#LookUpTableOpenFOAM	This option indicates the name of the folder in which the post-processed flamelet profiles will be stored
#NumberOfVariances	Number of points in the variance of mixture fraction space for look-up table construction
#StretchingFactor	Stretching factor along the variance of mixture fraction space

Table 1.2: Options in Data.inp file for OpenSMOKE_LookUpTable.sh

```
OpenSMOKE_LookUpTable.sh -kinetics "KineticScheme" -input "Data.inp" -
build-library
```

Output files are stored in the folder whose name is specified through the `#LookUpTableTest` options. In particular in this folder a series of `.bin` files, corresponding to the post-processed flamelet profiles can be found, together with a `LookUpTable.out` file containing additional data about the look-up table. These `bin` files will be used by the `rhoSimpleFoamFlamelets` solver. See Figure 1.6 for additional details.

1.4.3 Assembling

The post-processed flamelet profiles (`bin` files described above), need to be organized in shelves, before their use in `libOpenSMOKE`. Each shelf refers to a different value of enthalpy defect. The available shelves are collected in a main folder, which will be called `pdfLibrary` in the following. The `pdfLibrary` folder contains a `LookUpTable.out` files, in which the list of enthalpy defects (i.e. the list of shelves) is reported. Each enthalpy defect has a specific sub-folder (let's say `PDF-X`, where `X` is the enthalpy defect value), in which the `bin` files described in the previous section, together with the `LookUpTable.out` file, are included. The tree reported in Figure 1.6 refers to a typical look-up table containing different values of enthalpy defects.

1.4.4 Tutorial

This tutorial describes the generation of a non-adiabatic look-up table for a mixture H_2/air . It can be found in the `LookUpTable_Assembling` folder distributed with `libOpenSMOKE` library. Inlet temperatures are 295K and 294K, for fuel and oxidizer streams respectively. Only 3 enthalpy defects are accounted for (0, -50 and -100 kJ/kg); for each enthalpy defect 10 scalar dissipation rates are simulated (from $1e-6$ Hz to extinction). A β -PDF will be used in the mixture fraction space. The kinetic scheme to be adopted is the `PolimiH2_1006`, which is distributed together with the `libOpenSMOKE` library (in `utilities/kinetics/PreProcessed` folder).

1. Generation of flamelet profiles (Step01 folder)

- a) Three sets of flamelet profiles must be generated, corresponding to the 3 different enthalpy defects required. Let's start from the first value (0 kJ/kg), which means adiabatic conditions, typing the following command line in `Step01` folder:

```
OpenSMOKE_SteadyStateFlamelet.sh
-kinetics "../..../utilities/kinetics/PreProcessed/PolimiH2CO_1006"
-input "Data.inp"
-schedule "Operations.inp"
```

- b) Let's rename the folder containing the flamelet profiles:

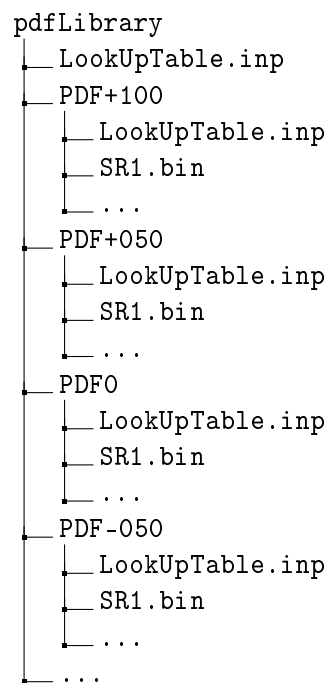


Figure 1.6: Look-up table structure

```
mv Flamelet_PolimiH2_1006/Profiles/ Flamelet-0
```

- c) Repeat the steps **a** and **b** also for the other 2 enthalpy defect values, by changing the `#EnthalpyDefect` line in the `Data.inp` input file and storing the flamelet profiles in `Flamelet-050` and `Flamelet-100` folders. At the end of these operations the generation of flamelet profiles is completed.

2. Post-processing (Step02 folder)

- a) Now we have to apply the β -PDF to the three sets of flamelet profiles we just created. Let's start from the adiabatic profiles in the `Flamelet-0` folder, by executing the `OpenSMOKE_LookUpTable` utility through the following command line in the `Step02` folder:

```
../../../../utilities/exe/OpenSMOKE_LookUpTable.sh  
-kinetics "../../../../utilities/kinetics/PreProcessed/PolimiH2_1006"  
-input "Input.inp"  
-build-library
```

At the end of this operation, the folder `PDF-0` will contain the post-processed flamelet profiles referring to adiabatic conditions (bin files and `LookUpTable.out` file).

- b) Then we have to repeat the operations in point **a** for the flamelets profiles in `Flamelet-050` and `Flamelet-100` folders. This can be accomplished by changing the list of flamelet profiles (`#ListOfFlamelets`) and the name of output folder (`#LookUpTableTableTest`). At the end of these operations three folders, `PDF-0`, `PDF-050` and `PDF-100`, will be available.

3. Look-Up table assembling

- a) The last step consist in assembling the folder containing the whole library. Create a folder with name `pdfFolder` (different names are possible) and put the three folders `PDF-0`, `PDF-050` and `PDF-100` in this folder.
- b) Create a new file in the `pdfLibrary` folder, called `LookUpTable.out`, in which the list of enthalpy defects must be written according to the following:

EnthalpyDefects

nphi 3

0. PDF-0

-50.e3 PDF-050

-100.e3 PDF-100

Each enthalpy defect (in J/kg) is followed by the name of the folder containing the corresponding binary files. The number of enthalpy defects is indicate by

the `nphi` option. The enthalpy defects in the list must be in decreasing order, otherwise an error message will be prompted out.

4. Final comments

If you want to extend the look-up table with new enthalpy defects, to cover a larger range or to be more accurate in some regions, you can add the corresponding new folders PDF-X and update the list of enthalpy defects in `pdfLibrary/LookUpTable.out` file.

1.5 Solvers

In this section a brief description of solvers available in `libOpenSMOKE` library is reported.

1.5.1 `rhoSimpleFoamFlamelets`

The `rhoSimpleFoamFlamelets` solver solves turbulent, non premixed flames using the steady-state, laminar flamelet model (SLFM), based on the RANS approach. Continuity and momentum equations are solved in the usual way together with three additional equations: mixture fraction (`csi`), variance of mixture fraction (`csiv2`) and enthalpy (`H`). The `rhoSimpleFoamFlamelets` solver needs a look-up in the format described in the previous section.

`flameletsProperties` Dictionary

The options to manage the SLFM are specified in the `flameletsProperties` dictionary. In Figure 1.7 an example is reported.

A first group of options is used to specify the main information about the management of look-up table:

- `libraryPath`: path to the folder containing the look-up table
- `adiabaticMode`: if this option is turned on the calculation is performed in adiabatic mode, even if the look-up table is non-adiabatic
- `varianceEquation`: if this option is turned off, the variance of mixture fraction is not transported, but calculated using an algebraic expression [13] (this saves computational time, but the predictions are expected to be less accurate)
- `propertyUpdate`: this option specifies the number of iterations to update the extractions of data from the look-up table. A large number saves computational time, but the stability of calculations can be negatively affected
- `massFractionsUpdate`: this option specifies the number of iterations to update the extractions of species from the look-up table. This number has no effect on the

```

//Flamelet Library
libraryPath "../PDF-Library";
adiabaticMode off;
varianceEquation on;
propertyUpdate 5;
massFractionsUpdate 50;
species "H2_OH_H2O_O2";

//Scalar Dissipation Rate PDF
pdf "dirac";
sigma 1.31;
points 30;

// Equation constants
sigmat 0.85;
Cg 2.86;
Cd 2.00;
Cx 2.00;

```

Figure 1.7: flameletsProperties dictionary

stability of calculations, since species mass fractions are not involved in the numerical solution, but are useful only for post-processing purposes

- **species:** list of species to be written on file for post-processing

The second group of options is used to specify the main features of scalar dissipation rate probability distribution:

- **pdf:** kind of probability distribution function to be used (**dirac** or **logNormal** options are available)
- **sigma:** variance of log-normal distribution (if **logNormal** option is turned on)
- **points:** number of discretization points in the mixture fraction space when **logNormal** option is turned on

The third group of options specifies the semi-empirical constants to be used in the transport equations:

- **sigmat:** Prandtl number in mixture fraction, variance of mixture fraction and enthalpy transport equations
- **Cg:** semi-empirical constant in transport equations
- **Cd:** semi-empirical constant in transport equations
- **Cx:** semi-empirical constant in transport equations

```

...
Calculate (first time)...
Fuel  enthalpy:      -43890.3 J/kg
Oxid. enthalpy:      -101000 J/kg
Fuel  temperature: 295 K
Oxid. temperature: 294 K
Preparing field rho (density)...
Preparing additional scalar fields (references)
...

```

Figure 1.8: Inlet values of enthalpy

Initial and boundary conditions

Initial and boundary conditions must be specified for pressure (p), velocity (U) and temperature (T) in the usual way. In addition initial and boundary conditions must be specified for the following variables:

- mixture fraction (csi): at fuel inlet mixture fraction is equal to 1, while at oxidizer inlet its value is equal to 0; at walls a **zeroGradient** condition must be specified;
- variance of mixture fraction ($csiv2$): at inlets variance of mixture fraction is usually equal to 0; at walls a **zeroGradient** condition must be specified;
- enthalpy (H): values of mass specific enthalpy at fuel and oxidizer inlets are required; this values can be read from video output when the **rhoSimpleFoamFlamelets** application starts (before the first iteration), as reported in Figure 1.8.

Output

Several fields are written in output folders:

- as : Planck mean absorption coefficient in $1/m$
- chi_st : scalar dissipation rate at stoichiometric condition in $1/s$
- csi : Favre-averaged mixture fraction
- $csiv2$: Favre-averaged variance of mixture fraction
- $epsilon$: Favre-averaged dissipation velocity turbulent kinetic energy in m^2/s^3
- H : Favre-averaged mass specific enthalpy in J/kg
- k : Favre-averaged turbulent kinetic energy in m^2/s^2

- `omega_YY`: Favre-averaged mass fraction of species YY
- `p`: pressure in Pa
- `phiH`: enthalpy defect in J/kg
- `Qrad`: radiative heat transfer in W/m^3
- `rho`: Reynolds-averaged density in kg/m^3
- `T`: Favre-averaged temperature in K

1.5.2 rhoPisoFoamFlamelets

The `rhoPisoFoamFlamelets` solver is the unsteady version of `rhoSimpleFoamFlamelets` solver described in the previous section. The input and output files are the same. The only difference is the definition of numerical schemes in `fvSolution` and `fvSchemes` dictionaries.

1.5.3 rhoSimpleFoamPostProcessor2E

The `rhoSimpleFoamPostProcessor2E` solver is used as a post-processor tool to estimate formation of soot in turbulent non premixed flames. It can be directly applied to the simulation results from `rhoSimpleFoamFlamelets` solver, but in principle it can be used on solutions obtained using different solvers. The `rhoSimpleFoamPostProcessor2E` can be applied using two different approaches:

- mean approach: solver needs as input the velocity (`U`), pressure (`p`), temperature (`T`) fields, together with composition fields of acetylene (`omega_C2H2`), oxygen (`omega_O2`), hydrogen (`omega_H2`), OH radical (`omega_OH`); no look-up tables are required;
- uncorrelated approach: solver needs as input the velocity (`U`), pressure (`p`) and temperature (`T`) fields, together with mixture fraction (`csi`) and variance of mixture fraction (`csiv2`).

In both cases two additional transport equations for soot particle number density (`phiN`) and soot mass fraction (`phiM`) are solved. Additional information is reported in Chapter 3.

sootPostProcessing Dictionary

In `sootPostProcessing` dictionary (Figure 1.9) the user can choose the main options for managing soot post-processing operations:

- `sigmat`: Prandtl number used in transport equations of `phiN` and `phiM`
- `sootUpdate`: number of iterations to update soot source terms in `phiN` and `phiM` equations

```

sigmat          0.85;
sootUpdate      5;
sootRobust      on;
sootClosure     "Uncorrelated";

nucleationModel "Liu_2002";
growthModel     "Liu_2002";
oxidationModel  "NSC";
aggregationModel "Smoluchowski";

libraryPath     "../PDF-Library-Soot";

```

Figure 1.9: Example of sootPostProcessing dictionary

- **sootRobust**: if this option is turned on, soot sink terms are evaluated using a more robust approach (this increases stability, but computational time is larger)
- **sootClosure**: closure approach for soot source terms (Mean and Uncorrelated options are available)
- **nucleationModel**: numerical model for nucleation of soot particles. Available options are: Liu_2001, Liu_2002, Moss_1999, Wen_2003, Lindstedt_1994 and Leung_1991.
- **growthModel**: numerical model for molecular growth of soot particles. Available options are: None, Liu_2001, Liu_2002, Moss_1999, Wen_2003, Lindstedt_1994 and Leung_1991.
- **oxidationModel**: numerical model for oxidation of soot particles. Available options are: None, Lee, NSC and Neoh.
- **aggregationModel**: numerical model for aggregation of soot particles. Available options are: None, Smoluchowski and Moss.
- **libraryPath**: path to folder containing the soot look-up table (only if sootClosure option is equal to Mean)

Initial and boundary conditions

Initial and boundary conditions must be specified for **phiN** and **phiM**. At inlet streams of fuel and oxidizer a fixed value must be specified. If the inlet streams are assumed soot free, it is suggested to use the inlet values reported on video when post-processing calculations are started (Figure 1.10).

```

...
OpenSMOKE_SootEmpiricalModels
Nucleation: 2
Growth: 2
Oxidation: 2
Aggregation: 1
Diameter (primary particles): 2.4 nm
Mass (primary particles): 8407.7 kg/kmol
Nuclei (primary particles): 700
PhiM(@1kg/m3): 1.92759e-11
PhiN(@1kg/m3): 2.29412e-15
...

```

Figure 1.10: Inlet values of phiM and phiN

Output

The following fields are written in output folders:

- fv: soot particles volume fraction
- dSoot: mean diameter of soot particles in m
- n0: number of soot particle per volume unit in $1/m^3$
- Sn: source term for phiN transport equation $kmol/m^3/s$
- Sm: source term for phiM transport equation $kg/m^3/s$
- Asoot: soot particle specific area in $1/m$

2 Flamelet Theory

The governing equations of steady laminar flamelets are reported and briefly discussed in the following. Some details about the numerical methods employed for their solution are given and the methodology adopted for the construction of the flamelet library is summarized.

2.1 Governing equations of laminar, steady flamelets

The steady laminar flamelet equations can be derived from the equations describing the counter flow diffusion flames, by adopting an appropriate transformation from the physical space to mixture fraction space (with Z as the independent variable). The mathematical procedure and the assumption needed for such transformation are described in [28] and [29] and are not here repeated. In the present approach a simplified set of the mixture fraction space equations is solved, according to the suggestions reported in [27]. In the following the conservation equations of species and energy in the mixture fraction space are reported:

$$\frac{1}{2}\rho\chi\frac{d^2\omega_k}{dZ^2} + \Omega_k = 0 \quad (2.1)$$

$$\frac{1}{2}\rho\chi\frac{d^2T}{dZ^2} - \frac{1}{C_P}\sum\hat{H}_k\Omega_k + \frac{1}{2C_P}\rho\chi\left[\frac{dC_P}{dZ} + \sum C_{P,k}\frac{d\omega_k}{dZ}\right]\frac{dT}{dZ} = 0 \quad (2.2)$$

The boundary conditions for the fuel (F) and oxidizer (O) sides are:

$$Fuel\ side\ (Z = 1) \quad \left\{ \begin{array}{l} \omega_k = \omega_{k,F} \\ T = T_F \end{array} \right. \quad (2.3)$$

$$Oxidizer\ side\ (Z = 0) \quad \left\{ \begin{array}{l} \omega_k = \omega_{k,O} \\ T = T_O \end{array} \right. \quad (2.4)$$

In the Equations reported above, χ is the scalar dissipation rate, which must be modeled across the flamelet. Several approaches are assumed. The most appropriate is an extension of a simpler expression [26] to variable density flows:

$$\chi(Z) = \frac{a_S}{4\pi} \frac{3\left(\sqrt{\frac{\rho_O}{\rho}} + 1\right)^2}{2\sqrt{\frac{\rho_O}{\rho}} + 1} \exp\left[-2\left(\operatorname{erfc}^{-1}(2Z)\right)^2\right] \quad (2.5)$$

where a_S is the characteristic strain rate, $erfc^{-1}$ is the inverse complementary error function and ρ_O is the density of the oxidizer stream.

2.1.1 Extension to non adiabatic combustion

The extension to non adiabatic combustion requires the introduction of the enthalpy defect ϕ_H , which is defined as the difference between the actual enthalpy \hat{H} and the enthalpy for an adiabatic flame:

$$\phi_H = \hat{H} - \left[\hat{H}_O - Z \left(\hat{H}_F - \hat{H}_O \right) \right] \quad (2.6)$$

where \hat{H}_O and \hat{H}_F denotes respectively the enthalpy of oxidizer and fuel streams. A set of laminar flamelets profiles, at different scalar dissipation rates, must be calculated at several fixed values of enthalpy defect. The profiles are organized in shelves, where each shelf contains entries referring to values of χ_{st} (scalar dissipation rate at stoichiometric conditions), ranging from equilibrium to extinction, plus the pure-mixing (or inert) state, and each shelf refers to a different value of enthalpy defect. Assuming the hypotheses of equal diffusivities, it is relatively easy to calculate the new flamelet profiles corresponding to the assigned enthalpy defect ϕ_H . If the same value of the enthalpy defect is enforced at both the fuel and oxidizer sides, the enthalpy defect is uniform across the whole flamelet. Many commercial codes assume that flamelet species profiles are unaffected by enthalpy defect, which means that for each enthalpy defect in the flamelet library the species profiles are assumed to be the same for the adiabatic flamelet; only the temperature profile is updated, using a simplified approach, which avoids to recalculate a new set of flamelets [24, 9]. The main disadvantage of this approach is that the effect of the heat losses on the species mass fractions is not taken into account. On the contrary, libOpenSMOKE utilities recalculate from scratch the flamelet profiles (both for temperature and mass fractions) for each enthalpy defect. This approach is very accurate, but requires the calculation of a very large number of laminar flamelet profiles. For example if ~ 10 enthalpy defects are considered and for each of them ~ 20 flamelet profiles are generated, the overall number of flamelets to be generated is ~ 200 .

2.1.2 Transient solution method

The overall model consists of a differential system of the conservation equations with boundary conditions for the dependent variables. The numerical solution of the overall system corresponding to differential equations (2.11) and (2.8) requires particular attention. In the present thesis the equations (2.11) and (2.8) are solved in a transient form, which is obtained by adding the corresponding time derivatives, in order to obtain a parabolic system of partial differential equations, rather than an ordinary differential equation boundary value system. The transient equations are reported in the following and are solved for a time which is long enough to reach steady state conditions:

$$\rho \frac{d\omega_k}{dZ} = \frac{1}{2} \rho \chi \frac{d^2 \omega_k}{dZ^2} + \Omega_k = 0 \quad (2.7)$$

$$\rho \frac{dT}{dZ} = \frac{1}{2} \rho \chi \frac{d^2 T}{dZ^2} - \frac{1}{C_P} \sum \hat{H} \Omega_k + \frac{1}{2C_P} \rho \chi \left[\frac{dC_P}{dZ} + \sum C_{P,k} \frac{d\omega_k}{dZ} \right] \frac{dT}{dZ} = 0 \quad (2.8)$$

2.1.3 Finite difference discretization

The equations reported above are discretized by means of a non uniform spatial grid, in order to obtain a system of ordinary differential equations. The adopted discretization uses conventional finite differencing techniques for non-uniform mesh spacing:

$$\frac{d\omega_{k,j}}{dZ} = \frac{1}{2} \chi_j \frac{\frac{\omega_{k,j+1} - \omega_{k,j}}{Z_{j+1} - Z_j} - \frac{\omega_{k,j} - \omega_{k,j-1}}{Z_j - Z_{j-1}}}{\frac{1}{2} (Z_{j+1} - Z_{j-1})} + \frac{\Omega_{k,j}}{\rho_j} = 0 \quad (2.9)$$

$$\begin{aligned} \frac{dT_j}{dZ} = \frac{1}{2} \chi_j \frac{\frac{T_{j+1} - T_j}{Z_{j+1} - Z_j} - \frac{T_j - T_{j-1}}{Z_j - Z_{j-1}}}{\frac{1}{2} (Z_{j+1} - Z_{j-1})} + \frac{\sum \hat{H}_{k,j} \Omega_{k,j}}{\rho_j C_{P,j}} + \\ \frac{\chi_j}{2C_{P,j}} \left[\frac{dC_P}{dZ} \Big|_j^{cen} + \sum C_{P,k} \frac{d\omega_k}{dZ} \Big|_j^{cen} \right] \frac{dT}{dZ} \Big|_j^{cen} = 0 \end{aligned} \quad (2.10)$$

where the first derivative are discretized using the central differencing scheme:

$$\begin{aligned} \frac{d\psi}{dZ} \Big|_j^{cen} = \psi_{j-1} \frac{Z_{j+1} - Z_j}{(Z_j - Z_{j-1})(Z_{j+1} - Z_{j-1})} + \\ \psi_j \frac{Z_{j-1} - 2Z_j + Z_{j+1}}{(Z_{j+1} - Z_j)(Z_j - Z_{j-1})} + \psi_{j+1} \frac{Z_j - Z_{j-1}}{(Z_{j+1} - Z_j)(Z_{j+1} - Z_{j-1})} = 0 \end{aligned} \quad (2.11)$$

2.2 Non adiabatic flamelet library construction

After flamelet generation, the flamelet profiles are convoluted with assumed-shape PDFs and then tabulated for look-up in the CFD code. The instantaneous value of any state quantity ψ inside a flamelet can be expressed as a function of the mixture fraction Z , the scalar dissipation rate χ_{st} and the enthalpy defect ϕ_H :

$$\psi = \psi(Z, \chi_{st}, \phi_H) \quad (2.12)$$

The corresponding mean value can be obtained by introducing the joint-PDF $P(Z, \chi_{st}, \phi_H)$:

$$\tilde{\psi} = \int_{-\infty}^{\infty} \int_0^{\infty} \int_0^1 \psi(Z, \chi_{st}, \phi_H) P(Z, \chi_{st}, \phi_H) dZ \cdot d\chi_{st} \cdot d\phi_H \quad (2.13)$$

In presumed PDF approach, a shape for the joint-PDF $P(Z, \chi_{st}, \phi_H)$ is assigned on empirical basis. Many experimental and numerical evidences [8, 26], indicated that mixture fraction and scalar dissipation rate are statistically independent. According to the suggestions proposed by Bray and Peters [10], the joint-PDF can be split in the product of three PDF's of a single variable:

$$P(Z, \chi_{st}, \phi_H) = P(Z) P(\chi_{st}) P(\phi_H) \quad (2.14)$$

According to Bilger [7], the result of integration with respect to the mixture fraction is relatively insensitive to the details of the PDF shape, if it is chosen on physical grounds. Usually a β -PDF or a clipped-Gaussian PDF are adopted. The integration with respect to χ_{st} is not a problem, as all evidence unanimously indicates a log-normal distribution for the shape of the associated PDF. The enthalpy defect PDF is usually assumed to be a Dirac delta function centered on the local mean value of enthalpy defect [23].

2.2.1 The β -PDF

The β -PDF is the most used approach for modeling the mixture fraction PDF, which is described by the following function:

$$P(Z) = \frac{Z^{a-1} (1-Z)^{b-1}}{\int_0^1 Z^{a-1} (1-Z)^{b-1} dZ} = \frac{\beta(Z)}{\int_0^1 \beta(Z) dZ} \quad (2.15)$$

where a and b are two non-negative parameters and are related to the mean \tilde{Z} and the variance of the mixture fraction $\widetilde{Z''^2}$, calculated by the solver:

$$a = \tilde{Z} \left[\frac{\tilde{Z} (1 - \tilde{Z})}{\widetilde{Z''^2}} - 1 \right] \quad (2.16)$$

$$b = (1 - \tilde{Z}) \left[\frac{\tilde{Z} (1 - \tilde{Z})}{\widetilde{Z''^2}} - 1 \right] \quad (2.17)$$

In general the distribution is asymmetric, but approaches a symmetric Gaussian shape when the ratios $\sqrt{\widetilde{Z''^2}}/\tilde{Z}$ and $\sqrt{\widetilde{Z''^2}}/(1 - \tilde{Z})$ are small.

2.2.2 The Clipped-Gaussian PDF

The clipped Gaussian PDF is based upon the clipping of a Gaussian function so that the probability is finite only in the allowable region of mixture fraction. A clipped Gaussian PDF contains a Gaussian distribution for the turbulent region $0 < Z < 1$ and Dirac delta functions for the intermittent appearance of unmixed fluid at $Z = 0$ and $Z = 1$. In Favre form it is given by:

$$P(Z) = a_1 \delta(Z) + (1 - a_1 - a_2) \frac{G(Z)}{I_G} + a_2 \delta(1 - Z) \quad (2.18)$$

where $\delta(Z - Z_0)$ is the Dirac delta function centered in $Z = Z_0$, whose integral is unity if $Z = Z_0$ and is zero otherwise; the variable I_G is defined as:

$$I_G = \int_0^1 G(Z) dZ \quad (2.19)$$

The unknown free parameters a_1, a_2 , and variance g of the Gaussian distribution, which are function of the mean \tilde{Z} and the variance of the mixture fraction $\widetilde{Z''^2}$, can be evaluated using the computationally inexpensive method suggested by Cleary [12]:

$$g = \min \left[\widetilde{Z''^2}, \left(\frac{\tilde{Z}}{2} \right)^2, \left(\frac{1 - \tilde{Z}}{2} \right)^2 \right] \quad (2.20)$$

$$G(Z) = \begin{cases} \frac{1}{\sqrt{2\pi g}} \exp \left(-\frac{(Z - \tilde{Z})^2}{2g} \right) & \text{for } \frac{|Z - \tilde{Z}|}{\sqrt{g}} \leq 2 \\ 0 & \text{for } \frac{|Z - \tilde{Z}|}{\sqrt{g}} > 2 \end{cases} \quad (2.21)$$

$$a_1 = \left(1 - \frac{\tilde{Z} (1 - \tilde{Z}) - \widetilde{Z''^2}}{\tilde{Z} (1 - \tilde{Z}) - g} \right) (1 - \tilde{Z}) \quad (2.22)$$

$$a_2 = \left(1 - \frac{\tilde{Z} (1 - \tilde{Z}) - \widetilde{Z''^2}}{\tilde{Z} (1 - \tilde{Z}) - g} \right) \tilde{Z} \quad (2.23)$$

2.2.3 The log-normal distribution

The log-normal distribution is largely used for describing the PDF of scalar dissipation rate:

$$P(\chi_{st}) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma \chi_{st}} \exp \left(-\frac{1}{2\sigma^2} \left(\ln \frac{\chi_{st}}{\widetilde{\chi_{st}}} - \frac{\sigma^2}{2} \right)^2 \right) \quad (2.24)$$

where it is assumed that $\sigma = 2$ (according to the experimental results by Sreenivasan et al. [31]).

Numerical integration

The numerical integration with respect to the enthalpy defect is straightforward, because the associated PDF is simply a Dirac delta function:

$$\begin{aligned}\tilde{\psi} &= \int_{-\infty}^{\infty} \int_0^{\infty} \int_0^1 \psi(Z, \chi_{st}, \phi_H) P(Z) P(\chi_{st}) \delta(\phi_H - \widetilde{\phi}_H) dZ \cdot d\chi_{st} \cdot d\phi_H = \\ &= \int_0^{\infty} \int_0^1 \psi(Z, \chi_{st}, \widetilde{\phi}_H) P(Z) P(\chi_{st}) dZ \cdot d\chi_{st} \quad (2.25)\end{aligned}$$

On the contrary, the numerical integration with respect to the mixture fraction and the scalar dissipation requires attention and must be performed in an accurate and inexpensive way:

$$\tilde{\psi} = \int_0^{\infty} P(\chi_{st}) d\chi_{st} \int_0^1 \psi(Z, \chi_{st}, \widetilde{\phi}_H) P(Z) dZ \quad (2.26)$$

Integration with respect to Z . Let us focus the attention on the evaluation of the integral $\int_0^1 \psi(Z, \chi_{st}, \widetilde{\phi}_H) P(Z) dZ$ with respect the mixture fraction. For the clipped Gaussian PDF the numerical evaluation of such integral is relatively simple, due to the absence of singularities and can be obtained using the usual quadrature formulas [16]. However, while the formulation of the β -PDF looks simple compared to the clipped Gaussian, the need to numerically determine the integral reported above can be computationally expensive. The numerical integration of the β -PDF encounters difficulties due to the singularity problem at either the oxidizer side (O) or the fuel side (F), depending on the parameters \mathbf{a} and \mathbf{b} , and the overflow problem when the PDF parameters are sufficiently large:

$$\int_0^1 \psi(Z, \chi_{st}, \widetilde{\phi}_H) P(Z) dZ = \frac{\int_0^1 \psi(Z, \chi_{st}, \widetilde{\phi}_H) \beta(Z) dZ}{\int_0^1 \beta(Z) dZ} \quad (2.27)$$

where $\beta(Z) = Z^{a-1} (1-Z)^{b-1}$. Liu et al. [19] suggested to evaluate the integrals at numerator and denominator by using the following approximate solution, which removes the singularities at the boundaries of the integration domain:

$$\begin{aligned}\int_0^1 \varphi(Z) \beta(Z) dZ &= \int_0^{\varepsilon} \varphi(Z) \beta(Z) dZ + \int_{\varepsilon}^{1-\varepsilon} \varphi(Z) \beta(Z) dZ \\ &+ \int_{1-\varepsilon}^1 \varphi(Z) \beta(Z) dZ \simeq \varphi_{ox} \frac{\varepsilon^a}{a} + \int_{\varepsilon}^{1-\varepsilon} \varphi(Z) \beta(Z) dZ + \varphi_{fuel} \frac{\varepsilon^b}{b} \quad (2.28)\end{aligned}$$

where ε is a small parameter (which is usually assumed to be 10^{-6}) and $\varphi(Z)$ is a generic function which corresponds to for the integral at numerator and to 1 for the integral at

denominator. The integral $\int_{\varepsilon}^{1-\varepsilon} \varphi(Z) \beta(Z) dZ$ can be now numerically calculated using the conventional quadrature formulas [16].

Integration with respect to χ_{st} . The integration with respect to χ_{st} is simpler to perform. In this work the approach suggested by Marracino and Lentini [23] is adopted. From the (2.29), after the integration with respect to Z :

$$\tilde{\psi} = \int_0^\infty P(\chi_{st}) d\chi_{st} \int_0^1 \psi\left(Z, \chi_{st}, \widetilde{\phi_H}\right) P(Z) dZ = \int_0^\infty H\left(\widetilde{Z}, \widetilde{Z''^2}, \chi_{st}, \widetilde{\phi_H}\right) P(\chi_{st}) d\chi_{st} \quad (2.29)$$

The integration range in χ_{st} is split into L sub ranges $[\chi_{l-\frac{1}{2}}; \chi_{l+\frac{1}{2}}]$, with $l = 1, 2, \dots, L$ and $\chi_{l-\frac{1}{2}} = 0$, such that χ_l can be considered a representative value for the corresponding interval. The integral is evaluated by the following approximation:

$$\begin{aligned} \int_0^\infty H\left(\widetilde{Z}, \widetilde{Z''^2}, \chi_{st}, \widetilde{\phi_H}\right) P(\chi_{st}) d\chi_{st} &= \sum_{l=1}^L \int_{\chi_{l-\frac{1}{2}}}^{\chi_{l+\frac{1}{2}}} H\left(\widetilde{Z}, \widetilde{Z''^2}, \chi_{st}, \widetilde{\phi_H}\right) P(\chi_{st}) d\chi_{st} \simeq \\ &\sum_{l=1}^L H\left(\widetilde{Z}, \widetilde{Z''^2}, \chi_{st}, \widetilde{\phi_H}\right) \int_{\chi_{l-\frac{1}{2}}}^{\chi_{l+\frac{1}{2}}} P(\chi_{st}) d\chi_{st} \quad (2.30) \end{aligned}$$

The approximate evaluation of the integral reported above is not computationally expensive and is accurate even with a limited number of points in the χ_{st} -space, contrary to the large number needed in the Z -space. Now we need to evaluate the integrals:

$$\int_{\chi_{l-\frac{1}{2}}}^{\chi_{l+\frac{1}{2}}} P(\chi_{st}) d\chi_{st} = \int_{\chi_{l-\frac{1}{2}}}^{\chi_{l+\frac{1}{2}}} \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma \chi_{st}} \exp\left(-\frac{1}{2\sigma^2} \left(\ln \frac{\chi_{st}}{\widetilde{\chi_{st}}} - \frac{\sigma^2}{2}\right)^2\right) d\chi_{st} \quad (2.31)$$

By introducing the running integration variable $\theta = \frac{1}{\sqrt{2}\sigma} \left(\ln \frac{\chi_{st}}{\widetilde{\chi_{st}}} - \frac{\sigma^2}{2}\right)$, the integral becomes:

$$\int_{\chi_{l-\frac{1}{2}}}^{\chi_{l+\frac{1}{2}}} \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma \chi_{st}} \exp(-\theta^2) d\chi_{st} = \frac{1}{\sqrt{\pi}} \int_{\theta_{l-\frac{1}{2}}}^{\theta_{l+\frac{1}{2}}} \exp(-\theta^2) d\theta \quad (2.32)$$

The integral reported above has an analytical solution, which is given by:

$$\frac{1}{\sqrt{\pi}} \int_{\theta_{l-\frac{1}{2}}}^{\theta_{l+\frac{1}{2}}} \exp(-\theta^2) d\theta = \frac{1}{2} \left[\operatorname{erf}\left(\theta_{l+\frac{1}{2}}\right) - \operatorname{erf}\left(\theta_{l-\frac{1}{2}}\right) \right] \quad (2.33)$$

where erf is the error function and:

$$\theta_{l\pm\frac{1}{2}} = \frac{1}{\sqrt{2}\sigma} \left(\ln \frac{\chi_{l\pm\frac{1}{2}}}{\widetilde{\chi_{st}}} - \frac{\sigma^2}{2} \right) \quad (2.34)$$

3 Soot post-processing

3.1 Method of moments

For a generic mono-dispersed number density function, the moment of order k is defined as:

$$m_k(\mathbf{x}; t) = \int_0^\infty \xi^k n(L; \mathbf{x}; t) dL \quad (3.1)$$

If Equation (3.7) is multiplied by ξ^k and integrated, the following balance equation for the moment of order k is obtained:

$$\frac{\partial \widetilde{m}_k(\mathbf{x}; t)}{\partial t} + \frac{\partial}{\partial x_i} [\widetilde{u}_i \cdot \widetilde{m}_k(\mathbf{x}; t)] = \frac{\partial}{\partial x_i} \left[\Gamma_t \frac{\partial \widetilde{m}_k(\mathbf{x}; t)}{\partial x_i} \right] + \widetilde{S}_k^m(\mathbf{x}; t) \quad (3.2)$$

The Standard Method of Moments (SSM) solves a set of transport equations for a number of significant moments of the distribution. This approach is feasible only if the source term $\widetilde{S}_k^m(\mathbf{x}; t)$ in Equation (3.11) can be written using the moments which are tracked. Unfortunately this is possible only for very simple systems or assuming particular forms of the particle size distribution.

3.1.1 Modeling of soot formation

The soot formation in turbulent flames is usually modeled using semi-empirical models for describing the main processes of nucleation, growth, coagulation and oxidation of soot particles. The corresponding rate expressions can be written in terms of soot volume fraction f_V (or mass fraction ω_{soot}) and total number density m_0 , assuming a mono dispersed distribution. Under such hypothesis the population balance equation can be conveniently solved through the Standard Method of Moments by considering only the moments of order zero m_0 and three m_3 (if particle size is chosen as the internal coordinate), which are directly related to soot particle number density and soot volume fraction. This approach is used for predicting soot formation in turbulent flames. A more accurate approach, which removes the restrictive hypothesis of mono dispersed particle size distribution is based on the Direct Quadrature Method of Moments (DQMOM).

Two additional transport equations are solved in a CFD code to predict soot formation and evolution: the first equation accounts for the transport of particle number density m_0 (which is the moment of zero order of the particle size distribution); the second equation describes the transport of the soot volume fraction f_V (which is related to the moment of

order three of the particle size distribution). The particles are assumed to be spherical and the size distribution simply represented by an average diameter d_P . In other words, the particle size distribution becomes a simple Dirac delta function, centered on the average diameter. As a consequence:

$$m_3 = \int_0^\infty L^3 n(L) dL = \int_0^\infty L^3 \delta(L - d_P) dL = d_P^3 \quad (3.3)$$

From the hypothesis of spherical shape it is relatively easy to obtain the relation between the soot volume fraction f_V and the moment of order three:

$$\omega_{soot} = \frac{\pi}{6} \int_0^\infty L^3 n(L) dL = \frac{\pi}{6} m_3 \quad (3.4)$$

Therefore a transport equation for the soot volume fraction is perfectly equivalent to a transport equation for the moment m_3 of the particle size distribution. The relation between the soot volume fraction and the particle diameter is explicitly reported below for convenience:

$$d_P = \sqrt[3]{\frac{6 f_V}{\pi m_0}} \quad (3.5)$$

For numerical convenience two density weighted variables are introduced: ϕ_N for the particle density and ϕ_M for the soot mass fraction [11]:

$$\phi_N = \frac{m_0}{\rho N_{AV}} \quad (3.6)$$

$$\phi_M = \frac{\rho_{soot} f_V}{\rho} \quad (3.7)$$

The transport equations for these variables are given by:

$$\bar{\rho} \frac{\partial \widetilde{\phi_N}(\mathbf{x}; t)}{\partial t} + \bar{\rho} \widetilde{u}_i \frac{\partial \widetilde{\phi_N}}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\Gamma_t \frac{\partial \widetilde{\phi_N}}{\partial x_i} \right] + \widetilde{S}_{m_0} \quad (3.8)$$

$$\bar{\rho} \frac{\partial \widetilde{\phi_M}(\mathbf{x}; t)}{\partial t} + \bar{\rho} \widetilde{u}_i \frac{\partial \widetilde{\phi_M}}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\Gamma_t \frac{\partial \widetilde{\phi_M}}{\partial x_i} \right] + \widetilde{S}_M \quad (3.9)$$

It is relatively easy to recognize in the variable ϕ_M the soot volume fraction ω_{soot} . The source terms can be written as a sum of different contributions:

$$\widetilde{S}_{m_0} = \widetilde{S}_{m_0}^{nucleation} + \widetilde{S}_{m_0}^{aggregation} \quad (3.10)$$

$$\widetilde{S}_M = \widetilde{S}_M^{nucleation} + \widetilde{S}_M^{growth} + \widetilde{S}_M^{oxidation} \quad (3.11)$$

Name	Reference
Liu_2001	[20]
Liu_2002	[19]
Moss_1999	[11]
Wen_2003	[33]
Lindstedt_1994	[34]
Leung_1991	[34]

Table 3.1: Kinetic parameters for nucleation model

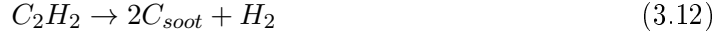
It is assumed that the influence of oxidation on the nucleation of soot particles is small and therefore the oxidation term is not included in the first equation [32].

For turbulent flames the effects of turbulent fluctuations should be taken into account in the evaluation of these source terms. The simplest approach, which has been followed by several authors [22, 33, 35], solves the transport equations and neglects the effects of turbulence.

3.2 Semi-empirical kinetic models

3.2.1 Nucleation Rate

Soot nucleation is described by the so called acetylene-route, which is based on a simple one-step reaction:



The corresponding source terms are expressed in the usual Arrhenius form:

$$S_{m0}^{nucleation} = A_{nucl} e^{-T_{nucl}/T} C_{C_2H_2} \quad (3.13)$$

$$S_M^{nucleation} = M_P S_{m0}^{nucleation} \quad (3.14)$$

In the expressions reported above A_{nucl} is the frequency factor, T_{nucl} is the activation temperature, $C_{C_2H_2}$ is the concentration of acetylene and M_P is the molecular weight of soot primary particles.

The user can choose between several semi-empirical constants for kinetic parameters reaction rates reported above. They are summarized in Table 3.1.

3.2.2 Growth Rate

According to Frenklach et al. [15], the soot particle growth is determined by the addition of acetylene and on the number of active sites on the surface. Assuming a mono-dispersed

Name	Area function	Reference
Liu_2001	$f = A_{soot}$	[20]
Liu_2002	$f = \sqrt{A_{soot}}$	[19]
Moss_1999	$f = A_{soot}$	[11]
Wen_2003	$f = A_{soot}$	[33]
Lindstedt_1994	$f = A_{soot}$	[34]
Leung_1991	$f = \sqrt{A_{soot}}$	[34]

Table 3.2: Kinetic parameters for growth model

spherical particle distribution, the soot specific surface area can be expressed as a function of the soot particle number density m_0 and to the soot volume fraction f_V :

$$A_{soot} = (36\pi)^{1/3} m_0^{1/3} f_V^{2/3} \quad (3.15)$$

The surface growth rate is given by:

$$S_{m0}^{growth} = A_{growth} e^{-T_{growth}/T} C_{C2H2} f(A_{soot}) \quad (3.16)$$

A range of area dependencies have been proposed in the literature; according to the most common approaches the function f is assumed linearly proportional to the soot specific surface area $f = A_{soot}$ or to square root surface area $f = \sqrt{A_{soot}}$. Although the square-root dependence of the soot surface area does not seem physically correct, it can be related to the surface aging phenomena and active-site surface deactivation [20].

Available growth models are summarized in Table 3.2

3.2.3 Coagulation Rate

The coagulation rate depends on soot particles density; assuming a mono-dispersed distribution of spherical particles:

$$S_{m0}^{aggregation} = \beta m_0^2 \quad (3.17)$$

According to Brookes and Moss [11] and Syed et al. [32], β is related to the temperature:

$$\beta = \frac{A_{aggregation}}{N_{AV}^2} \sqrt{T} \quad (3.18)$$

where $A_{coagulation}$ is a semi-empirical constant. The value proposed by Brookes and Moss [11] is used.

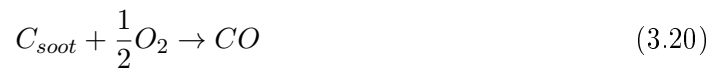
3.2.4 Oxidation Rate

The oxidation rate strongly depends on the hydroxyl radical (OH) and O₂ but also O radical can play an important role. The rate of oxidation is usually assumed proportional to the soot specific surface area:

$$S_{m0}^{oxidation} = \dot{m}_{ox} A_{soot} \quad (3.19)$$

Lee model

The model of Lee et al. [18] can be adopted and soot oxidation is described using a one-step reaction:



The soot oxidation term takes the form:

$$\dot{m}_{ox} = A_{ox} e^{-T_{ox}/T} \frac{PO_2}{\sqrt{T}} \quad (3.21)$$

This model was also used by Liu et al. [21], Wen et al. [33] and Ma et al. [22] and implicitly assumes that soot oxidation in a diffusion flame is controlled by O₂ into the zone of active soot oxidation at temperatures high enough to react with H and form OH, which is recognized as the main oxidizing species in the stoichiometric/lean side of the flame. On the contrary, O₂ becomes more important as any surviving particles enter oxygen-rich regions where temperature is still high [14].

NSC model

The model of proposed by Nagle and Strickland-Constable [25] assumes that the reaction rate is given by the following expression:

$$\dot{m}_{ox} = 120 \left[\frac{k_A P_{O_2}}{1 + k_Z P_{O_2}} \chi + k_B P_{O_2} (1 - \chi) \right] \quad (3.22)$$

where:

$$\chi = \frac{1}{1 + \frac{k_T}{k_B P_{O_2}}} \dot{m}_{ox} \quad (3.23)$$

The kinetic constants k_A , k_B , k_T and k_Z can be found in [25, 34]

3.3 Closure of soot source terms

One of the major issues in the modeling of soot formation is the closure of the soot source terms in the conservation equations for soot particle number density m_0 and soot volume fraction f_V . In general the mean source term can be expressed using the proper joint-PDF $P(Z, \chi_{st}, \phi_H, m_0, f_V)$:

$$\tilde{S} = \int_0^\infty \int_0^\infty \int_{-\infty}^\infty \int_0^\infty \int_0^1 S(Z, \chi_{st}, \phi_H, m_0, f_V) P(Z, \chi_{st}, \phi_H, m_0, f_V) dZ \cdot d\chi_{st} \cdot d\phi_H \cdot dm_0 \cdot df_V \quad (3.24)$$

The form of this joint-PDF is unknown, both experimentally and theoretically, and therefore simplified approaches must be used in order to obtain the closure of the source term.

3.3.1 Mean Properties

The simplest approach consists in evaluating the source term using the mean flame properties and totally ignoring the effects of turbulence [11]. In this case the joint-PDF can be split in the product of five PDFs of a single variable:

$$P(Z, \chi_{st}, \phi_H, m_0, f_V) \approx P(Z) P(\chi_{st}) P(\phi_H) P(m_0) P(f_V) \quad (3.25)$$

Moreover each PDF simply becomes a Dirac delta function centered on the mean value of each independent variable:

$$P(Z, \chi_{st}, \phi_H, m_0, f_V) \approx \delta(Z - \tilde{Z}) \delta(\chi_{st} - \tilde{\chi}_{st}) \delta(\phi_H - \tilde{\phi}_H) \delta(m_0 - \tilde{m}_0) \delta(f_V - \tilde{f}_V) \quad (3.26)$$

3.3.2 Uncorrelated closure

A different solution assumes that mixture fraction and enthalpy defect are completely uncorrelated with soot properties (m_0 and f_V). This solution was adopted by many authors [1, 11, 30] and assumes that the influence of scalar fluctuations in the gas phase are dominant. The joint-PDF can be split in the product of two different PDFs:

$$P(Z, \chi_{st}, \phi_H, m_0, f_V) \approx P(Z, \chi_{st}, \phi_H) P(m_0, f_V) \quad (3.27)$$

Moreover, the soot properties are also assumed statistically independent:

$$P(Z, \chi_{st}, \phi_H, m_0, f_V) \approx P(Z, \chi_{st}, \phi_H) P(m_0) P(f_V) \quad (3.28)$$

The single PDF for the soot volume fraction is unknown. Two Dirac delta functions can be used to obtain the closure. The final form of the joint-PDF is therefore the following:

$$P(Z, \chi_{st}, \phi_H, m_0, f_V) \approx P(Z, \chi_{st}, \phi_H) \delta(m_0 - \widetilde{m}_0) \delta(f_V - \widetilde{f}_V) \quad (3.29)$$

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