Flamelet Model for OpenFOAM®-2.2.x

Introduction

The flamelet model build by Alberto Cuoci – called libOpenSMOKE – is generated for OpenFOAM®-1.7.x. In my masterthesis I used that model in the Release 2.1.x. For that I asked Bruno Santos for help. He rebuild the whole flamelet model for OpenFOAM®-2.1.x. Therefor I want to thanks Bruno again for his perfect work. A year ago I was not able to build thermodynamics in OpenFOAM®. He gave me the ability to work with that model and learn a lot of new things – especially developement.

In the new OpenFOAM® Version (2.2.x) there are some changes in the thermophysical classes. For that its not possible to build the old flamelet thermophysical model into the new version. Hence it is necessary to rebuild the thermophysical model.

This brief description gives you an overview about the changes and how to use the model.

Changes

In the new model there are some changes and new options avaiable.

- Option to show the initialization of the flamelet library
- Option to monitor important variables while calculation
- Rename the variables
- Clean the flamelet thermophysical model

Variables

Favre averaged variables:

- **Z**: mixture fraction
- **Zvar**: variance of mixture fraction
- **H**: mass specific enthalpy [J/kg]
- **defect**: enthalpy defect [J/kg]
- **chi_st**: scalar dissipation rate [1/s]
- **omega_YY**: mass fraction of species YY

- **Qrad**: radiative heat transfer [W/m^3]

Reynolds averaged variables:

- **rho**: density [kg/m^3]

Non averaged variables

- **as**: planck mean absorption coefficient [1/m]

Initial and boundary conditions

Initial and boundary conditions must be specified for pressure (p), velocity (U) and temperature (T) in the usual way. Further more you have to specify the following variables:

- mixture fraction (**Z**): at fuel inlet the value of Z is equal to 1, while at oxidizer inlet its value is equal to 0. At walls a zeroGradient must be specified.
- varianz of mixture fraction (**Zvar**): at the inlets (fuel+oxidizer) its set to 0; at walls set zeroGradient.
- enthalpy (**H**): values of mass specific enthalpy at fuel and oxidizer inlets are required; Set the values to the adiabatic enthalpy. This value can be read from the output when **flameletSimpleFoam** application starts the first time, as reported in Listing 1.1. If you want to specify a wall with fixed temperature (enthalpydefect) set the same BC equal to 0.

```
1  Thermo flamelet set the adiabat enthalpy for enthalpy defect calculation:
2
3    + Adiabat enthalpy fuel: -2.19608e+06
4    + Adiabat enthalpy oxidizer: -17992.9
```

Listing 1: Output message for the adiabatic specific enthalpy

thermophysical model

There is only one thermophysical model avaiable called **flameletThermo**, simply because the calculation of all thermo variables are calculated in the flamelet build operation. The entry in the **thermophysicalProperties** is given in Listing 1.2:

```
1  thermoType
2  {
3      type            pdfFlameletThermo;
4      mixture         pureMixture;
5      transport       sutherland;
6      thermo          hConst;
7      equationOfState perfectGas;
8      specie          specie;
9      energy          sensibleEnthalpy;
10 }
```

Listing 2: Output message for the adiabatic specific enthalpy

flameletProperties dictionary

The new version provides new options. You can use the features setting the right variables in the **flameletProperties** dictionary in the constant folder. The new dictionary is listed below.

```
1       //- Path to flamelet library
2       libraryPath                     "PDF-Library";
3
4       //- Output modes
5       showFlamelet                    off;
6       showFlameletLibrary             off;
7
8       //- Show Z, Zvar and H (min/max)
9       monitoring                      off;
10
11      //- Adiabatic mode
12      adiabaticMode                   off;
13
14      //- Radiation model (only for free stream flames)
15      radiationMode                   on;
16
17              //- Environment temperature
18              Tenv                    Tenv            [0 0  0 1 0 0 0]   292.15;
19
20      //- Algebraic eqn. for mixture fraction variance
21      varianceEquation          off;
22
23      //- LookUpTable extraction after <n> iterations
24
25              //- Thermo variables
26              propertyUpdate                  5;
27
28              //- mass fraction
29              massFractionsUpdate             50;
30
31      //- Species that are saved for paraview
32      species                         "CO H2 H2O O2 N2 CO2 OH";
33
34      //- Scalar Dissipation Rate PDF
35
36              //- Kind of calculation (dirac|logNormal)
37              pdf               "dirac";
38
39              //- Options for logNormal
40              //- Splitting Zvar with expanson factor
41              sigma             1.31;
42
43              //- Integration intervals (Z)
44              points            50;
45
46      //- Equation constants
47      sigmat            0.85;
48      Cg                2.86;
49      Cd                2.00;
50      Cx                2.00;
51
52
53      //- Turbulence: k-e model
54      k_small                 k_small         [0 2 -2 0 0 0 0]   1.e-6;
55      epsilon_small           epsilon_small   [0 2 -3 0 0 0 0]   1.e-6;
```

Listing 3: flameletProperties dictionary

Contact and information

If you want to know how to build your flamelets and transform them into a Look-Up-Table you should have a look into the official User-Guide; included in the doc dictionary.

If you want more information or think this model should be improved you can send me an Email:
Tobias.Holzmann@Holzmann-cfd.de
or be updated
http://creckmodeling.chem.polimi.it/

If you think this very brief description should contain the whole calculation methods send me an Email: Tobias.Holzmann@Holzmann-cfd.de

If there are some people who want build an own open source flamelet generate, I will work with you.

If you want to thank for the rebuild you can support me with money (: