Short introduction to the modified libOpenSMOKE libraries

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1 Introduction

The documentation gives a short overview about the steady-state laminar flamelet model (SLFM) created by Alberto Cuoci et al.. Further more the modifications I made are given in the sections below.

The solvers and libraries are tested and validated in my masterthesis with the SANDIA CO/H2/N2 flame. Therefor adiabatic and non-adiabatic mode was used and compared. Further more I made an benchmark in a complex biomass burning chamber with results from ANSYS-CFX® and measurements. Here you should know that the flamelet-solver gives good quality results but the quantity result is not good to predict species mass fraction.

For a better convergence I build the flamelet-solver with the SIMPLEC algorithm that allows you to get better results and a stabilization in your calculation due to the pressure-corrected-equation [8].

The following solvers are avaiable for OpenFOAM® 2.1.x:

- turbulentFlameletRhoSimpleFoam
  its the same solver like in Alberto's tool
- turbulentFlameletRhoSimplecFoam
  using the SIMPLEC algorithm

The following scripts are avaiable:

- runFlameletGeneration.sh
  automatic generation of flamelet libraries with different enthalpy defects

Notice

The model gives good results with free-stream flames but there is no warranty for the correctness of that libraries, results and my modifications.

2 Steady-State Laminar Flamelet Model

This chapter gives a short introduction into the flamelet-model. At the beginning the flamelet generation is discussed. After that the transport equations are given.

2.1 Flamelet Generation

The steady-state laminar flamelet model is a combustion model based on the mixture fraction. Its possible to describe every physical value ϕ with the mixture fraction Z. You simplify the combustion to the conserved scalar Z. For that you have to generate *flamelets*. They describe the flame structure. Additionally you need the scalar dissipation rate χ; that is like an inversed time scale. The following expression shows the correlation between the parameters in laminar diffusion flames:

$$\phi = f(Z, \chi) \quad . \tag{2.1}$$

If you want to describe turbulent flows you have to extend the flamelets. First every variable is splitted into the mean value and its fluctuation:

$$Z = \bar{Z} + Z', \qquad \chi = \bar{\chi} + \chi' \quad . \tag{2.2}$$

By using RANS-modelling you have to average the values:

$$\bar{Z} = \overline{\bar{Z} + Z'}, \qquad \bar{\chi} = \overline{\bar{\chi} + \chi'} \quad . \tag{2.3}$$

The result is the following:

$$\bar{Z} = \bar{\bar{Z}} + \bar{Z}', \qquad \bar{\chi} = \bar{\bar{\chi}} + \bar{\chi}' \quad . \tag{2.4}$$

In the litrature the fluctuation is often given by $\bar{Z}''$ instead of $\bar{Z}'$. For that reason the fluctuations are given by the modifier $''$.

Changing Eq. (2.1) to turbulent flows and introducing the enthalpy defect ϕ_H for non-adiabatic systems you get the following correlations:

$$\bar{\phi} = f(\bar{Z}, \bar{Z}'', \bar{\chi}, \bar{\chi}'', \bar{\phi}_H, \bar{\phi}_H'') \quad . \tag{2.5}$$

Now its necessary to combine the variables Z to $\bar{Z}, \bar{Z}''$, χ to $\bar{\chi}, \bar{\chi}''$ and ϕ_H to $\bar{\phi}_H, \bar{\phi}_H''$. This is managed by introducing probability distribution functions. For the mixture fraction it can be shown that the β-PDF gives a good result. Considered to the scalar dissipation rate the log-Normal-function is used. At least the analyses of the defect gives the δ-function. All probability functions are independend and can be calculated seperate. The equation that must be solved is given below:

$$\tilde{\phi} = \int\int\int \phi(Z, \chi, \phi_H)\ \tilde{P}(Z, \chi, \phi_H)\ \mathrm{d}Z\ \mathrm{d}\chi\ \mathrm{d}\phi_H \quad , \tag{2.6}$$

and produces the Look-Up-Table ensemble. Notice that the calculation use the favre weighted expression. Eq. (2.6) is solved by the binaries build by Alberto Cuoci. For more information have a look at the references.

While the algorithm is calculate the the numerical solution, the thermo model extract all necessary variables out of the Look-Up-Tables. With the values of $\tilde{Z}, \tilde{Z}'', \tilde{\chi}$ and $\tilde{\phi}_H$ you can extract the values $\tilde{\phi}$. Therefor you are using an area weighted interpolation scheme. Thats the reason why the fluctuation of the mixture fraction must be normalized to the limits [0:1] equal to the mixture fraction so that the projection of the 3D-surface to the $\tilde{Z}$-$\tilde{Z}''$-plane are rectangles.

2.2 Transport equations

Using the flamelet model you have to implement the transport equation for the mixture fraction $\tilde{Z}$, the fluctuation of the mixture fraction $\tilde{Z}''$ and the calculation of the scalar dissipation rate $\tilde{\chi}$. For non-adiabatic system you need the information of the enthalpy-defekt and it is necessary to add a transport equation for the enthalpy $\tilde{H}$.

mixture fraction:

$$\cancelto{0}{\bar{\rho}\frac{\partial \tilde{Z}}{\partial t}} + \underbrace{\bar{\rho}\tilde{\mathbf{v}} \cdot \nabla \tilde{Z}}_{\text{convection}} = \underbrace{\nabla(\bar{\rho} D \nabla \tilde{Z} - \bar{\rho}\widetilde{\mathbf{v}''Z''})}_{\text{diffusion}} \quad .$$

varianze of mixture fraction:

$$\cancelto{0}{\bar{\rho}\frac{\partial \tilde{Z}''}{\partial t}} + \underbrace{\bar{\rho}\tilde{\mathbf{v}} \cdot \nabla \tilde{Z}''}_{\text{convection}} = \underbrace{\nabla(\bar{\rho} D_{\mathrm{t}} \nabla \tilde{Z}'')}_{\text{diffusion}} + \underbrace{2\bar{\rho} D_{\mathrm{t}} (\nabla \tilde{Z})^2}_{\text{1. QT}} - \underbrace{\bar{\rho}\tilde{\chi}}_{\text{2. QT}} \quad .$$

enthalpy:

$$\cancelto{0}{\bar{\rho}\frac{\tilde{H}}{\partial t}} + \underbrace{\bar{\rho}\mathbf{v} \cdot \nabla \tilde{H}}_{\text{convection}} = \underbrace{\nabla\left(\frac{\mu_{\mathrm{t}}}{\sigma_{\mathrm{t}}} \nabla \tilde{H}\right)}_{\text{diffusion}} \quad ,$$

scalar dissipation rate:

$$\tilde{\chi} = 2D(\nabla \tilde{Z})^2 = C_\chi \frac{\tilde{\epsilon}}{\tilde{k}} \tilde{Z}'' \quad .$$

The enthalpy equation has to be modified. The reason is, that Alberto‘s tool can use a fixed temperature wall BC for describing heat loose effects. The problem therefor is, that the turbulent diffusion is zero if you are on a wall. Similiar is the convection term equal zero. In my thesis it is shown that there is no information exchange between the walls and the fluid region. Hence it is necessary to implement the μ_{eff} into the diffusion term. The modified enthalpy equation is:

enthalpy:

$$\cancelto{0}{\bar{\rho}\frac{\tilde{H}}{\partial t}} + \underbrace{\bar{\rho}\mathbf{v} \cdot \nabla \tilde{H}}_{\text{convection}} = \underbrace{\nabla\left(\mu_{\text{eff}} \nabla \tilde{H}\right)}_{\text{diffusion}} \quad ,$$

3 Modifications

- Update the enthalpy-equation with the effectiv viscosity to describe heat looses on walls.
- Option to switch on/off the radiation model. That is necessary couse the radiation model is valid only in free-stream flames. The problem is, that you set the ambience temperature to a fixed value. In complex burning chambers the model gives wrong enthalpy values. You can switch the radiation model on/off in the flameletPropertiesDict.
- The user may set a fixed inlet temperature for the fuel and oxidizer. If you do so, the thermomodel produces wrong results caused by the fixed wall temperature BC. Due to the fixed temperature the adiabatic enthalpy at the inlets will be overwritten by the thermomodel and leads to wrong enthalpy-defect calculation. Thats a fatal error. Its not a bug couse you do not have to set the temperature for the inlets but for that case that the user do it, I implemented some lines in the thermo model that fix the problem.
- Added the flamelet model into the SIMPLEC algorithm for a better convergence and stabilization during the calculation of p and U.
- Added the flamelet model into the PIMPLE algorithm for using transient calculations.
- Added a script for easy building non-adiabatic Look-Up-Tables automatically.
- Added tutorials that shows a validation case of an CH4/N2/H2 flame and a non-adiabatic burning geometry.

4 Case setup

This chapter showes you how to set up a case correct. The variables are:

- U - velocity
- p - pressure
- k - turbulent kinetic energy
- epsilon - dissipation rate (for turbulence)
- csi - mixture fraction
- csiv2 - mixture fraction varianz
- chi_st - scalar dissipation rate
- H - enthalpy
- T - temperature
- as - planck mean absorption coefficient (for radiation)
- omega_YY - mass fraction of species YY

4.1 Adiabatic mode

If you wish to calculate an adiabatic system you have to set up your case like a normal OpenFOAM® case. For the inlets define csi with fixedValue. The value is 1 for the fuel inlet and 0 for the oxidator inlet. The variable csiv2 is fixedValue with 0 on both inlets. The enthalpy has fixedValues too. At the inlet BC you have to set the adiabatic enthalpy. The value is shown in the terminal by starting the flamelet solver. Further more you can set your temperature values to the inlet; that is not necessary.

4.2 Non-Adiabatic mode

If your simulation is a free-stream flame you can switch on the radiation model by setting the *radiationMode* variable in the flameletPropertiesDict to *on*. Otherwise you should turn the model off and work with fixed temperature walls. Therefor you have to set the temperature wall to a fixed value and the same BC in the enthalpy file H *must* be set to fixedValue too. The value you set is not important couse the model overwrite the value in the first iteration.

4.3 Tutorials

For creating flamelets and kinetic files have a look at [6]. For setting up a correct case have a look into the tutorials.

4.4 Parameters and output

In both solvers I impmlemented an output-section that shows you the minimum and maximum values of the following variables:

- density $\tilde{\rho}$
- mixture fraction $\tilde{Z}$
- varianz of mixture fraction $\tilde{Z}''$
- enthalpy $\tilde{H}$.

You should know that the mixture fraction is limited to the intervall [0:1]. For the varianz $\tilde{Z}''$ the value is limited between [0:0,25]. The thermomodel can handle other values but if you get i.e. $\tilde{Z}''_{max} = 24,242$ you should check your mesh, BC and/or relax factors. The output gives you the information if something is wrong with your setup or mesh.

If you are using adiabatic mode the enthalpy $\tilde{H}$ is not used in the calculation but the minimum and maximum values should be the adiabatic values for the fuel and oxidator stream. Its just a notice to the user if everything is working fine.

5 Compiling the libraries

To use the modified libraries and solvers switch into your *$WM_PROJECT_USER_DIR* and execute the following command in your terminal:

```
git clone https://github.com/shor-ty/flameletModel.git
```

After that switch into the directory and execute the compilation script by typing the following command into the terminal:

```
cd flameletModel
./compileAll
```

If you want to compile everything by ourself go into the libraries and compile the libs step by step:

```
cd flameletModel/libraries
cd common
wmake libso
cd ../flamelet/turbulent
wmake libso
cd ../../pdfThermo
wmake libso
```

After the libraries are compiled successfully you can compile the solver step by step:

```
cd flameletModel/applications
cd turbulentFlameletRhoSimpleFoam
wmake
cd ../turbulentFlameletRhoSimplecFoam
wmake
cd ../turbulentFlameletRhoPimpleFoam
wmake
```

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