Project 6: Equilibrium and Flamelet Modelling of Non-Premixed Turbulent Flames

Part A: Equilibrium Model

The purposes of this exercise are: for you to learn to set up the Nonpremixed, Equilibrium model in Fluent; to examine the equilibrium properties calculated by Fluent; and to examine the significance of mixture fraction fluctuations.

1. Read the relevant parts of Ch.15 of the Fluent 6.2 documentation. Focus on the simplest case of a single mixture fraction, adiabatic, with the equilibrium model.

2. Set up Fluent for the Sandia/ETH hydrogen jet flame using the equilibrium model. Do so by following the instructions in Project 5, Part B, Ex.2, but (in 2(c)) set up the Species Transport yourself, instead of reading the journal file `pdf_equil.jou`. Include the following species (and only these species) in this order: H_2, N_2, O_2, O, H, OH, HO_2, H_2O, H_2O_2.

3. Examine the PDF table produced (Display → PDF Table/Curves...). For the stoichiometric value of mixture fraction, compare the equilibrium temperature and mass fraction of OH with that given by EQUIL. Report your findings.

4. Exit Fluent; run fluent 2ddp and read in the Case & Data file `BC_Ce1_16.cas.gz`. This is the same as in Project 5, using the standard k-ε model, except that the model constant $C_{\varepsilon 1}$ is changed to 1.6. Check that the solution is converged. Read in the Journal file `export_radial.jou`, and save the resulting file (with the first line removed) as `Post/radial_base.dat`. Use the Matlab script `Post/he0.m` to examine the results. Note that more quantities are plotted than in Project 5.

5. In order to examine the influence of mixture fraction fluctuations, set the value of the model constant C_g to zero. Do so by typing `(rpsetvar 'cgvar 0)` in the text user interface (TUI). This sets the production of scalar variance to zero, so that the converged solution has zero scalar variance. Iterate to convergence; verify that the scalar variance is very small; and use `export_radial.jou` to generate the file of radial profiles (`Post/radial_Cg0.dat`, say). Use `Post/he0.m` to compare the results to the base case. Report the profiles of mean temperature.

6. Make a list of all of the sources of discretization error involved in these Fluent calculations. How can each one be reduced?

7. What are the principal assumptions in the equilibrium model? Where in this flame are they most likely to be inaccurate?

Part B: Flamelet Model

The purpose of this exercise is to use the flamelet model to make calculations of the Sandia/ETH flame, and to compare the results to those from the equilibrium model.

1. Read Ch.15.3 of the Fluent 6.2 User Guide. Using `fluent 2ddp` and starting from the Case & Data file `BC_Ce1_16.cas.gz`, follow the instructions in the User Guide to set up the flamelet model for the Sandia/ETH flame. To do so, use the Chemkin mechanism file `RD_H2_a.inp`. Set the maximum number of flamelets to 100. How many flamelets are generated? What is the maximum scalar dissipation? What is the maximum temperature in this flamelet?

2. Examine the properties of the flamelets generated. Plot T vs. ξ and the mole fraction of OH vs. ξ for the two flamelets with the lowest and highest values of scalar dissipation. (Hint: under Display → PDF Tables/Curves..., select "2D Curve on 3D Surface".)

3. Iterate to convergence. Read in the Journal file `export_radial.jou`, and save the resulting file (with the first line removed) as `Post/radial_flamelet.dat`. Use the Matlab script `Post/he0.m` to compare the results of the equilibrium and flamelet models. (Note that the ordering of the species is different for the flamelet model than for the equilibrium model; and the variables `KFLA` and `KFLB` in the Matlab script must be set accordingly.) Comment on your observations.

4. In the model equation for the mixture fraction variance $g \equiv \widetilde{\xi''^2}$, the mean scalar dissipation is modelled as
$$\tilde{\chi} = C_d g \frac{\varepsilon}{k}. \tag{1}$$
Note that (with the flamelet model) $\tilde{\chi}$ is available in the Display and Plot menus, under "Pdf". What is the maximum value of $\tilde{\chi}$ in the solution domain? Where does it occur? Does the centerline value vary with axial distance (approximately) as a power law?

5. According to the steady laminar flamelet model, a burning flamelet cannot exist for $\chi \geq \chi_q$, where χ_q is the quenching value of the scalar dissipation. Assume that χ is log-normally distributed, with $\mathrm{var}(\ln(\chi/\tilde{\chi})) = 2$; and define χ_α such that for $\tilde{\chi} = \chi_\alpha$, $\mathrm{Prob}(\chi > \chi_q) = \alpha$.

   Optional: show that χ_α is given by
$$\chi_\alpha = \chi_q \exp(1 + 2\mathrm{erf}^{-1}(2\alpha - 1)), \tag{2}$$
   and hence $\chi_{0.1}/\chi_q = 0.444$, and $\chi_{0.9}/\chi_q = 16.7$.

   Not optional: For this flame, report the values of $\chi_{0.1}$ and $\chi_{0.9}$. Use contour plots to identify the regions where (a) $\mathrm{Prob}(\chi \geq \chi_q) > 0.9$ and (b) $\mathrm{Prob}(\chi \geq \chi_q) > 0.1$

(Note: although this is not stated in the documentation, in Fluent, when χ exceeds χ_q, flamelet values are taken from the burning flamelet with the largest value of χ, i.e., $\chi \approx \chi_q$.)