Project 7: Transported Composition PDF Method

Lifted Turbulent Jet Flame in a Vitiated Co-Flow

An experiment has been performed by Cabra et al. (2002) on a H_2/N_2 jet issuing into a hot (1045K) vitiated co-flow. In this exercise, the Composition PDF Transport model is used to make calculations of this flame. In order to keep the computational time requirements within reasonable bounds, the calculations are performed on a very coarse grid, and other simplifications are made, and so the results are not numerically accurate.

1. Visit the web site `http://www.me.berkeley.edu/cal/VCB/Data/` to gain an understanding of the experiment. Note the experimental configuration, the states of the streams, and the observed lift-off height.

2. Read the of Ch.17 of the Fluent 6.2 documentation.

3. Set up Fluent for the Cabra jet flame using the Composition PDF Transport Model. Do so through the following steps:

   (a) Run `fluent 2d` and read in the mesh file `cabra4.msh`. The units used in generating the mesh are mm. Go to Grid → Scale and set "Units Conversion" appropriately. Then "Scale" and "Close". Display the grid, note the number of cells, and understand the definitions of the different "Surfaces". (Note: as part of the simplification of the problem, the fuel tube wall is treated as a symmetry boundary — the grid is not fine enough to resolve the boundary layer.)

   (b) Change the solver to "Axisymmetric". Select the standard k-ε turbulence model.

   (c) Import the Chemkin mechanism `Li_noCO.inp`. (This is just the Li mechanism, with unnecessary species removed.)

   (d) Select the Transported Composition PDF method (Define → Species → Transported Species.) At this stage do NOT turn on volumetric reactions.

   (e) Set appropriate boundary conditions. Boundary conditions need to be set for `coflow` and `jet`. For `coflow` set the axial velocity to 3.5 m/s, the turbulence intensity to 2%, the lengthscale to 0.005 m, the temperature to 1045 K, $Y_{O_2} = 0.17$, and $Y_{H_2O} = 0.07$. For the `jet`, set the axial velocity to 107 m/s, the turbulence intensity to 10%, the hydraulic diamter to 0.005 m, the temperature to 305 K, and $Y_{H_2} = 0.0233$.

   (f) Set the residual monitors to be plotted. Reduce the Convergence Criterion for x-velocity to 10^{-6}. Set a monitor for the average temperature on `outlet1`. Save the Case.

   (g) Set initial conditions by: Solve → Initialize → Initialize... → Compute From `coflow`.

4. A converged solution can best be obtained in several stages. The intermediate solution should be examined after each stage.

   (a) Turn off the solution of Pdf in Solve → Controls → Solution..., so that only Flow and Turbulence are being solved. Iterate to convergence.

(b) In Solve → Controls → Solution, turn on the solution of Pdf, and reduce the number of particles per cell to 10. Iterate until the temperature monitor indicates that the solution is statistically stationary (e.g., a further 300 iterations). (Note that volumetric reactions are turned off at this stage. The residuals will not decrease significantly because of the statistical noise in the mean density.)

(c) Examine contour plots of mean axial velocity, mean temperature, and mean OH. Make scatter plots of the particles, color coded by particle temperature, and by particle mass fraction of OH. To do this, go to Display → Particle Tracks..., check the box "Track PDF Transport Particles", and under "Color by" select Particle Variables, and Particle Temperature, etc.

(d) In Define → Models → Species → Transport & Reaction, turn on Volumetric Reactions. In Integreation Parameters, change the ISAT tolerance to 0.0002, the Max. Storage to 500, and Verbosity to 2. Set all "Discretizations" to "Second Order Upwind". Iterate until a statistically stationary stae is achieved (about 100 furthet iterations). (After 10 iterations, you may want to check that a non-trivial, burning solution is being obtained: a scatter plot of OH will reveal if ignition is occurring.) Save the Case & Data.

5. Make a contour plot of mean OH. Note that the base of the flame is about 5 mm off the axis. Add a "Surface" named `r5`, corresponding to the line y = 5mm. (Surface → Iso-Surface.) Along this line, and along the axis, plot against x: the mean axial velocity, the mean temperature, and mean mass fraction OH and other species.

6. Create Custom Field Functions corresponding to: the mean mixture fraction $\tilde{\xi}$; the r.m.s. mixture fraction $\xi' \equiv \sqrt{\widetilde{\xi''^2}}$; the turbulence frequency $\omega \equiv \varepsilon/k$; and the modelled mean scalar dissipation $\tilde{\chi} \equiv 2\xi'^2\varepsilon/k$. To define $\tilde{\xi}$ and ξ', note that ξ is linearly related to Y_{N_2}. Examine contour plots of these quantities. Make plots of them along the axis and along the line `r5`.

7. Make a scatter plot color coded by mean OH (not particle OH) with the grid displayed. Zoom in on the base of the flame, including a portion of the upstream region. Then (in the same window) make a plot of the particle OH. Comment on your observations.

8. Increase the number of particles per cell to 20; set the Time Average Increment to 0.5 (in Solve → Iterate); and iterate for as long as your patience allows. Comment on how the monitored quantities vary.

9. Perform one iteration using Direct Integration instead of ISAT. (Define → Species → Transport & Reaction, Integration Parameters. Note that this will clear the ISAT table.) Measure the CPU time required for this iteration (e.g., by recording the CPU time shown in Task Manager before and after the iteration). Report you result in seconds, and also expressed as micro-seconds per particle.

10. Suppose that you had unlimited computational power at your disposal. Itemize the steps you would take to improve the accuracy of the solution.

11. The file `isat_stats.out` generated while running Fluent contains information about the performance of ISAT. Read the Fluent User Guide to understand its contents. Run the Matlab script `fisat2.m` which post-processes `isat_stats.out`. Report the average CPU time in ISAT per query (in μs) over the whole run, and also over the final reporting interval. Compare these numbers for the corresponding figure for Direct Integration. (You may also

examine the file `isat_stats_long.out` which comes from a fairly long run of this case on a slow laptop.)

12. Make a calculation of the same flame using one of the other models available in Fluent. Compare basic results with the Transported PDF calculations and comment on your observations.