Project 5: Simple Chemistry and Turbulence Modelling using Fluent

Part A: Simple chemistry

The purpose of this exercise is to learn to use Fluent to perform simple chemistry and flame calculations, and to compare the results with Chemkin.

1. The files `aurora_H2.inp` and `RD_H2_a.inp` can be used to run CHEMKIN IV for a case of hydrogen/air auto-ignition. The objective of this exercise is to run the same case in Fluent. You can do this through the following steps.

   (a) At a command prompt in an appropriate directory, enter `fluent 2ddp`

   (b) Read in the mesh file `square.msh`. (File → Read → Case). Display the grid. What is it?

   (c) Import the Chemkin mechanism `RD_H2_a.inp` (File → Import→ Chemkin Mechanism). Change the "Material Name" to RD-H2-a.

   (d) By default, Fluent solves steady problems. In Define → Models → Solver, set "Time" to "Unsteady".

   (e) Go to: Define → Models → Species → Transport & Reaction, and turn on Species Transport; turn on Volumetric Reactions; turn on Stiff Chemistry Solver. Under "Integration Parameters", set all three tolerances to 10^{-10}.

   (f) Under Define → Models, check that all other settings are appropriate.

   (g) Under Define → Materials, change "Density" to "ideal-gas".

   (h) Under Solve → Initialize → Initialize, set the appropriate initial conditions. (Note that pressure is "gauge pressure"; species are in mass fractions; and that the mass fraction of the last species, N_2, is implied.)

   (i) In Solve → Monitors → Residual, under Options, turn on "plot".

   (j) In Solve → Monitors → Volume, make the appropriate settings to plot and write temperature versus time.

   (k) Save the Case & Data (File → Write → Case & Data) as `auto_H2.cas.gz`.

   (l) In Solve → Iterate, set the time step size to $10^{-5}s$, the number of steps to 50, and iterate. Note the final temperature.

   (m) Compare the results from Fluent to those from CHEMKIN IV.

2. Use Fluent to make a Plug Flow Reactor calculation based on the same conditions as in Exercise 1. This can be done as follows.

   (a) use the mesh file `duct.msh`. What is this? What boundary types are specified?

   (b) import the Chemkin mechanism.

   (c) set up Species Transport as before: set the ISAT error tolerance to 10^{-6}, leave the ODE error tolerances unchanged.

(d) set inlet boundary conditions corresponding to a stream at 100m/s with the same thermochemical properties as in the autoignition case.

(e) set initial conditions; set monitors; iterate to convergence.

(f) make changes as necessary to obtain a numerically accurate solution.

(g) run CHEMKIN IV under the same conditions (i.e., constant pressure and enthalpy) and compare the results. (Note that $u\,dx$ in the PFR corresponds to dt in autoignition.)

3. In this exercise, Fluent is used to make a calculation of a laminar premixed flame. The geometry is polar cylindrical (x-r), with variation in the r-direction only. The solution domain extends from $r_{\min} = 5$cm to $r_{\max} = 7$cm, with $r = r_{\min}$ being an inflow boundary at which the velocity is specified ($V(r_{\min}) = 2.8$ m/s).

   (a) Start `fluent 2ddp`.

   (b) Read in the mesh file `flame2.msh` and inspect the grid.

   (c) Import the Chemkin mechanism `chem_H2.inp` and the transport database `tran.dat`.

   (d) In Define → Solver, under "Space" select Axisymmetric.

   (e) Turn on: Species Transport; Volumetric reactions; stiff chemistry solver; and set the ISAT error tolerance to 10^{-6}.

   (f) Set the inlet boundary conditions: $V = 2.8$ m/s, $T = 300K$, $Y_{H_2} = 0.0283$, $Y_{0_2} = 0.2264$, $Y_{A_r} = 0.01$.

   (g) In Solve → Controls → Solution, set the discretization to second order upwind.

   (h) Set initial conditions, monitors, save the case and iterate to convergence.

   (i) Plot density, velocity and the mass fractions of H_2, H, O and OH against temperature, and compare to the values obtained from CHEMKIN IV.

Part B: Turbulence Modelling

The purpose of this exercise is to explore the performance of the various turbulence models applied to the Sandia/ETH hydrogen/air turbulent non-premixed flame.

1. Visit the web site: `http://www.ca.sandia.gov/TNF/DataArch/H2HeData.html` which describes the flame to be studied. (Here we are interested only in the flame with pure hydrogen fuel.) Understand the flow geometry, boundary conditions, and the available experimental data.

2. In this part, you set up Fluent for the Sandia/ETH flame using the standard $k - \varepsilon$ model.

   (a) Run `fluent 2d` and read in the mesh file `r250.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 and understand the definitions of the different "Surfaces". Hint:de-select all of the "default-interiors" and display the grid.

   (b) Change the solver to "Axisymmetric. Select the $k-\varepsilon$ turbulence model with "Enhanced Wall Treatment".

   (c) Read in the journal file (File → Read → Journal...): `pdf_equil.jou`. This sets up the chemistry, which we will study in the next project. You can go to Define → Models → Species → Transport & Reaction to see the settings,but do not change anything.

(d) Under Define → Operating Conditions, set Gravity appropriately.

(e) Set appropriate boundary conditions. Boundary conditions need to be set for the following surfaces: coflow, coflow2, fuel, outlet, outlet2; but you should check that the remaining surfaces are indeed set correctly. In the co-flow(2), set the turbulence intensity to 2% and the lengthscale to 0.002 m. At outlet(2),conditions should be set in case backflow occurs: setting $k = 10m^2/s^2$ and $\varepsilon = 200m^2/s^3$ is reasonable.

(f) Set appropriate initial solution. This setting can strongly affect the rate of convergence of the iterations. Reasonable settings (in SI units)are: $U = 1$, $k = 0.01$, $\varepsilon = 10$, $\xi = 0$.

(g) Set the residual monitors to be plotted. Reduce the Convergence Criterion for x-velocity to 10^{-5}. Set a monitor for the average temperature on "outlet".

(h) An accurate converged solution can best be obtained in several stages.

i. Turn off the solution of Pdf in Solve → Controls → Solution..., so that only Flow and Turbulence are being solved. Do 100 iterations.

ii. Turn on the solution of Pdf, and iterate until reasonably converged (maybe a further 600 iterations).

iii. Improve the solution by changing the "discretization" to PRESTO! for pressure, and "Second Order Upwind" for all other quantities.Reduce the Under-Relaxation Factor for density to 0.5. Iterate until convergence is again obtained (maybe a further 400 iterations).

(i) Compare the calculated center-line velocity with the experimental data.

3. Exit Fluent, and run fluent 2ddp. Read in the Case & Data file `BC_base`. This is essentially the same case as set up in the previous question, but some surfaces have been added for facilitate post-processing. These surfaces,which can be viewed via Display → Grid, correspond to the axial locations at which the experimental data are available. Compare the center-line profile of mean axial velocity with the solution you obtained in the previous question.

   In the sub-directory Post, the Matlab script `he0.m` compares radial profiles from two Fluent calculations with the experimental data. As may be seen from the start of this script, the Fluent output files are of the form `radial_ABC.dat` where "ABC" designates the particular case.

   In Fluent, read the journal file `export_radial.jou`. This generates the output file radial.dat containing information on the radial profiles. (Check that a new version of this file is indeed created.) Examine this file in a text editor, remove the first line, and save the modifed file in the Post directory with an appropriate name, e.g.,Post
   `radial_base.dat`.

   In Post, run the Matlab script `he0.m` with both cases being the base case, i.e., FLA = `radial_base.dat` and FLB = `radial_base.dat`. Examine the plots produced.

4. In order to examine the dependence of the calculations on the turbulence model constants: change the value of $C_{\varepsilon 1}$ to 1.6; iterate to convergence; read the journal file `export_radial.jou`; edit and re-name the resulting file; and run the Matlab script to compare the results with the base case and with the experimental data.

5. Explore the performance of one of the other turbulence models in Fluent, namely:

   (a) Spalart-Allmaras

(b) $k - \varepsilon$ RNG

(c) $k - \varepsilon$ Realizable

(d) Reynolds-Stress Model: standard

(e) Reynolds-Stress Model: SSG

(f) Reynolds-Stress Model: LRR-IP

(g) Reynolds-Stress Model: LRR-QI

(h) Reynolds-Stress Model: Jones-Musonge

Compare two calculations: one with the default values of the turbulence-model constants; and one with $C_{\varepsilon 1}$ modified so that the calculated mean velocity on the center-line at $x/L = 1/2$ is in approximate agreement with the experimental data.