ME6170 Project
Unsteady Perfectly Stirred Reactors

Due: April 29 5pm

Submission: A zipped package with matlab code and report. Email to: tlu@engr.uconn.edu

Project description

Step 1: read the notes on stirred reactors posted online. Derive the equations for unsteady PSR for given residence time and initial conditions. Ignore the terms related to surface reactions and heat loss.

Step 2: read the provided template for solving ODEs and figure out the differences between implicit and explicit solvers. The implicit solver is required for chemical reacting flows.

Step 3: modify the template to solve unsteady PSR for methane-air with different initial conditions. Use the CKWYP function in the updated matlab toolbox to compute the species production rates.

Test cases:

1. Starting from fuel-air mixture at $T_{in} = T_{out} = 1200K$, p = 1atm and $\phi = 0.5$, solve the temperature and species concentrations for different resident time, $\tau = 1\ \mu s, 1ms, and\ 1s$, respectively. Make sure you get a solution on the upper branch for the long resident time.

2. Use the solution on the upper branch as the initial condition, solve the temperature and species profiles for $\tau = 1\mu s$, make sure that extinction occurs.

Bonus: Formulate the steady state PSR systems and write a program to solve the algebraic equations using fsolve or fzero. You need to normalize the variables and equations very carefully to get converged solutions. If successful, use the program to obtain an S-curve for methane air. Perturb the steady state solution and use the unsteady code to compute how temperature and species concentrations change with time for points on the upper and middle branches, respectively.