MMJ 1443 Advanced Combustion
July 2009/2010

Project 1

Aim: In this project, you are going to plot the concentration of species vs. time to see how species are produced and destroyed over time.

Specifics: You will be studying the thermal NOx mechanism as given below (this is also given in Chapter 5 of your text). Set up a system of simultaneous ordinary differential equations that describes the reaction rates of the various species. Use Matlab to solve this system of ODE's. Solve for an initial condition where only N_2 and O_2 exist with an equal concentration. Assume the whole reaction occurs at 2000K and 1 atm. Use your own judgment to determine the duration, t, that you want to study the reaction progress.

Deliverables: Your report should include the description of the problem, how you set up the problem, assumptions, method of solution, the Matlab code that you used, the results, the plot (all species on one graph), discussion and potential weaknesses in your solution method. Hand in your report on a CD. If you want to use MS Word, use version 2003 or below (in .doc format and NOT .docx)

Hint: You can refer to Rao's Applied Numerical Methods book (your text for Computational Methods course) for examples on how to program Matlab to solve simultaneous ODE problems. The scans of the relevant pages are posted on my website.

The **thermal** or **Zeldovich mechanism** consists of two chain reactions:

$$O + N_2 \Leftrightarrow NO + N \qquad (N.1)$$

$$N + O_2 \Leftrightarrow NO + O, \qquad (N.2)$$

The rate coefficients for N.1–N.3 are [22]

$$k_{N.1f} = 1.8 \cdot 10^{11} \exp[-38{,}370/T(K)] \qquad [=]\, m^3/kmol\text{-}s,$$

$$k_{N.1r} = 3.8 \cdot 10^{10} \exp[-425/T(K)] \qquad [=]\, m^3/kmol\text{-}s,$$

$$k_{N.2f} = 1.8 \cdot 10^{7}\, T \exp[-4680/T(K)] \qquad [=]\, m^3/kmol\text{-}s,$$

$$k_{N.2r} = 3.8 \cdot 10^{6}\, T \exp[-20{,}820/T(K)] \qquad [=]\, m^3/kmol\text{-}s,$$