

AME 598I

Homework 1

Due: Friday, 24 January 2003, in class

Consider the problem of Oxygen dissociation and recombination that was performed in lecture.

1. Write a code in either Fortran or C to reproduce the results obtained in lecture for initial concentrations  $[\hat{O}_2] = 0.001 \text{ mol/cm}^3$ ,  $[\hat{O}] = 0.001 \text{ mol/cm}^3$ ,  $T = 5000 \text{ K}$  for the two step mechanism using reactions 13 and 14 in the CTM paper found in the documents section of the course home page. Give plots of concentration versus time and pressure versus time. You can compare your results to those obtained via the mathematica code for this problem which is available in the documents section of the course home page. I have placed an example Fortran code and matlab plotting code of the documents home page which you can use as a template. The example Fortran code happens to solve a mass spring damper system using the robust ODE solver, `dsode`, which is included.
2. For the same initial conditions, generate a plot of how the equilibrium concentrations of  $O$  and  $O_2$  vary with temperature.
3. For the same initial conditions, generate a plot of how the time scale of reaction near equilibrium varies with temperature. This time scale can be obtained by linearizing the system near equilibrium and examining the solution near the equilibrium point.