AME 60636
Prof. J. M. Powers
Homework 4
Due: Friday, 13 February 2009

Consider the ozone reaction mechanism given by Powers, Singh, and Paolucci, 2002, *Journal of Chemical Physics*, Vol. 117, p. 1482-1496. This is available in the documents section of the course website under the link "JCP slow manifold paper." Take the system to be isothermal with $T = 3000\ K$ and isochoric. At $t = 0\ s$, we have mass fractions $Y_O = 0.25$, $Y_{O_2} = 0.25$, $Y_{O_3} = 0.5$ and $P = 100\ kPa$. Take $V = 1\ m^3$.

1. Show that this mechanism is identical to that given by Margolis, 1978, *Journal of Computational Physics*, Vol. 27, p. 410. This will essentially require proper unit conversions and interpretations of nomenclature.
2. Find the density ρ and molar concentrations $\overline{\rho}_i$ at $t = 0\ s$.
3. Write a system of three ordinary differential equations in three unknowns to describe the evolution of each species concentration. Include appropriate initial conditions.
4. Find conserved quantities, and give the physical significance of each.
5. Reduce the system to two ordinary differential equations in two unknowns, where the unknowns are $\overline{\rho}_O$ and $\overline{\rho}_{O_3}$.
6. Find all equilibrium states, and identify which are physical.
7. Perform a local linear analysis around each physical equilibrium, and identify the time scales of reaction.
8. Write a Fortran 77 (or equivalent) codes to integrate the full equations from the initial state to the equilibrium state. Include a copy of your codes (leaving out the dlsode subroutine) as an appendix to your solution.
9. Plot all species concentrations versus t, being careful to elucidate all the time scales in the system.
10. Plot $\overline{\rho}_O$ versus $\overline{\rho}_{O_3}$.
11. Plot $P(t)$.
12. Estimate the enthalpies at the end states and calculate the total heat transfer in kJ in the process.