AME 598i Prof. J. M. Powers Homework 4 Due: Thursday, 17 February 2005

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 $Y_O = 0.25$, $Y_{O_2} = 0.25$, $Y_{O_3} = 0.5$ and p = 100 kPa. Take $V = 1 \text{ m}^3$.

- 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 c_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 [O] and $[O_3]$.
- 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 [O] versus $[O_3]$.
- 11. Plot p(t).
- 12. Estimate the enthalpies at the end states and calculate the total heat transfer in kJ in the process.