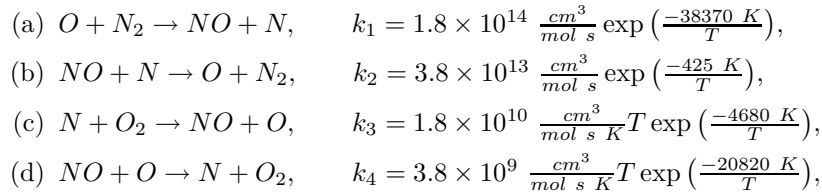


AME 598i
Prof. J. M. Powers
Homework 2
Due: Friday, 31 January 2003

1. Write a description of less than one page of the Zeldovich mechanism of NO_x production. Use the L^AT_EX text formatter to generate your output. Include appropriate formatted equations and appropriate references.
2. Consider a system which is a part of the Zeldovich mechanism for formation NO :



Take the system to be isothermal with $T = 1600\ K$ and isochoric with $V = 1000\ cm^3$. At $t = 0\ s$, we have $N_N = 1\ mol$, $N_{NO} = 2\ mol$, $N_{N_2} = 3\ mol$, $N_O = 4\ mol$, $N_{O_2} = 5\ mol$.

- Write a system of five ordinary differential equations in five unknowns to describe the evolution of each species concentration. Include appropriate initial conditions.
- Find conserved quantities and give the physical significance of each.
- Reduce the system to two ordinary differential equations in two unknowns, where the unknowns are $[O_2]$ and $[N_2]$.
- Find all equilibrium states, and identify which are physical.
- Perform a local linear analysis around each physical equilibrium, and identify the time scales of reaction.
- Write a Fortran 77 (or equivalent) code to integrate the full equations from the initial state to the equilibrium state. Include a copy of your code (leaving out the `dlode` subroutine) as an appendix to your solution.
- Plot all species concentrations versus t .
- Plot $[N_2]$ versus $[O_2]$.
- Plot $P(t)$.
- Using the thermochemical calculator (<http://blue.caltech.edu/tcc>) to estimate the enthalpies at the end states, calculate the total heat transfer in kJ in the process.