ChE 641
Review for Midterm Exam

Equilibrium Concepts

- why use it
- kinetic view of equilibrium
- K_{eq}
- ΔG^0
- getting K_{eq} and ΔG^0 as f(T)
- getting Y_i^{eq} from K_{eq}
- effects of T & P
- multiple species and reactions (minimize G)
  - constraints
- equilibrium codes (I/O, capabilities, potential uses)
  - Nasa-CEA
  - GasEQ
  - Cantera
- solids
  - biomass, coal
  - how to get ΔH_f^0

Chemical Mechanism Concepts

- Where can you find mechanisms
- How were mechanisms validated
- Associated thermo file

Chemical Reactor Concepts

PSR & Plug
- assumptions
- derivation of equations
- modes of operation
- networking reqactors

Premixed Reactor & Flame Mechanics
- assumptions
- derivation of equations
- diffusion of species and temperature
- operating procedures
- potential uses of ideal reactor codes (big picture)

Numerical Methods Involved
- Stiffness
- Newton method
- Jacobian matrix
- reverting to time-dependent solution

Sensitivity Analysis
- method and use

Partially-Stirred Reactor
- concept
- derivation
- potential uses

Types of Questions

- ✓ Use the code (NASA-CEA, GasEQ, Cantera, PSR, Batch, Plug)
- ✓ Interpret the output from a code
- ✓ Describe the numerical method of how a code works
- ✓ Show/derive the starting equations
- ✓ Simple hand calculations (at least set up) for equilibrium (using K_{eq})
- ✓ Explain the differences between codes
- ✓ Explain how a certain reactor might or might not be approximated by one of these simple application codes

- ✓ When to use equilibrium vs. a chemical reaction code (i.e., Cantera)