Chemical Engineering 522

Combustion Processes

Review 1

Exam 1 Review

- Classes 1-16 (plus review)
- Chapter 1
  - Introduction
- Chapter 2
  - Stoichiometry
  - Thermochemistry
  - Equilibrium
- Chapter 3
  - Mass transfer
- Chapter 4
  - Combustion Kinetics
- Chapter 5
  - Combustion Mechanisms
- Chapter 15
  - NOx

•Reading: Chps 1-5, 15

•Homework assignments 1-4

•Class discussions

Study Excercise

- Write down the main topic/title of each class
  - Try without the schedule, then with it
- For each class, what were the main ideas
  - Outline each class.
  - Put in details
  - What examples were done?
- Do this alone, then with others.
- Create your own review notes (like these slides).
  - First “recall” then look up to fill in.

Study Exercise

- Go back through the homework.
- Read the problem statements and think through the problems
  - What concepts are needed?
  - What is the approach used?
- Outline the the solution
- Don’t spend too much time trying to rework problems, but get the essense of the problem and try to do it from memory.

Study Exercise

- Write out simple examples of concepts and problems and how/why we did them.
- Do the same for key numerical tools considered.
- “Play professor,” what would you put on the exam? Try inventing your own problems.

Introduction

- Syllabus
- Schedule
- Handouts
- Introductions
- Combustion Overview
  - Fundamentals
  - Fuels
  - Pollutants
  - Applications

Combustion Basics, Flames

- Definition and characterization of combustion
- Premixed Flames
  - Intrinsic velocity
  - Intrinsic thickness
  - Basic propagation mechanism
- Nonpremixed flames
  - No flame speed
  - Arbitrary flame thickness
- Balance between diffusion and reaction

Energy and pollutants

- Energy use and energy density
- Combustion Issues
  - land, resources,
- 3 cubic miles of oil
- Pollutants (NO_x, SO_x, PM, metals)
- IPCC Climate Change
  - Temperatures, sea level, snow cover
  - CO_2, CH_4, N_2O,
  - Radiative forcings
  - Climate models

Stoichiometry

- Air composition, MW
- N_2/O_2 ratio, Air/O_2 ratio
- MW in terms of x_i
- MW in terms of y_i
- Convert x_i to y_i
- Stoichiometry
  - Equivalence ratio (know definition)
  - Mixture fraction (know definition)
  - General stoichiometric reaction for hydrocarbon combustion to products of complete combustion. (know the formula and how to get it).
  - Rich reaction: use equivalence ratio
  - Lean reaction: use excess air: $E=(1-\phi)/\phi$

Excess air example

- These are general principles; you should be able to use them to apply to similar but different systems.
  - Like, what if the fuel has sulfur or nitrogen; what if we specify incomplete products

Mixture Fraction

- Definition
  - In terms of streams
  - Relate to E.R.
  - "flame coordinate"
  - "conserved scalar"
- Compute ξ for a given composition
- Compute ξ_{st}
- PCC are linear in ξ

$$\xi = \frac{m_f}{m_f + m_o}$$

$$\phi = \frac{\xi}{1-\xi}\frac{1}{(F/A)_{st}}$$

$$\phi = \frac{\xi(1-\xi_{st})}{\xi_{st}(1-\xi)}$$

$$\psi = (\xi)(\psi)_{\xi=1} + (1-\xi)(\psi)_{\xi=0}$$

$$\xi = \frac{\psi - \psi_{\xi=0}}{\psi_{\xi=1} - \psi_{\xi=0}}$$

Adiabatic Flame Temperature

- ΔH_{comb}, ΔH_{rxn}
- HHV, LHV
- Basis: per mole, or per mass of mixture or per mass of fue
- Adiabatic flame temperature (constant P)

$$H_{react} = H_{prod} = \sum_i n_i h_{f,i} + \int_{T_r}^{T_{ad}} \sum_i n_i C_{p,i} dT$$

You should know this

  - know how to solve by hand, on computer.
  - Simple forms, and general forms.
  - How does T_{ad} changes with reactant temperature.
  - PCC versus equilibrium
- Constant volume flame temperature?
  - How to formulate?
  - How much different?

Equilibrium 1

- Dissociation products: CO_2, CO, H_2O, H_2, O_2, Fuel, N_2, H, OH, O, NO, N
- Major/minor species
- Criteria for equilibrium (how/why).
- Four case types
  - Adiabatic versus const T,P, or const T,V.

you should know this rxn

- WGS dissociation: $CO + H_2O = CO_2 + H_2$
  - By hand:
    - write combustion reaction → moles products are unknowns
    - elemental balances (how many)
    - equilibrium constraint
  - How good is it?
  - Where is it valid, where not?

Equilibrium 2

- Gibbs energy minimization
  - Element potential method.
  - Understand basics of how it is formulated and solved.
    - Minimize Gibbs
    - Elemental constraints
    - These two give N_{sp} equations in N_{sp} + N_{el}
    - Elemental constraint equations give Nel eqns.
    - Solve Nsp equations for ni and sub into constraint equations. (also have one for total moles)
    - Solve for lambdas, then solve for species.
    - Initial guess for lambdas from initial guess for species

Applications/Fuel Properties

- Otto cycle (4 strokes)
  - PV diagram
  - Net work from state of points on PV diagram.
  - Can do by hand if not full equilibrium.
- Diesel cycle
  - compare to Otto cycle.
  - How do diesel engines differ from SI (spark ignition) engines.
- Octane rating
- Exhaust gas recirculation
  - purpose/effects
- Recuperation/regeneration
  - purpose/effects

Mass Transfer

- Species versus Average versus diffusion velocities
- Different kinds of average velocities
- Constraint on fluxes
- General Fick's law discussed
  - matrix form: that is each species diffuses due to all other species gradients.
- Simplified Fick's law:
  - species diffuses due to own gradient only
  - Mole fractions or mass fractions? Convert from mole to mass form
- Diffusion coefficients: T, P dependence (know this)
- 1-D species equation
- Stefan problem: properties and analysis

Combustion Kinetics

- Elementary versus global reactions
  - rate law, reaction rate of species, reaction orders, bimolecular, third body species, etc.
  - Global reaction orders, limitations
- Compact notation
  - Summations, matrix form
  - Generic reaction, with coefficient matricies
  - H_2/O_2 example
  - Generic forward rates
  - Generic reverse rates
  - rate of progress variable q
  - rate of reaction for species in terms of q
- reverse reaction rates

Combustion Mechanisms

- QSSA, Partial equilibrium
  - How they work, what they accomplish
- Chain reactions, chain branching reactions
- General 4 step (3 step) H.C. oxidation scheme
- 3 reaction types (know examples, properties)
  - Initiation reactions
  - Chain reactions
  - Termination reaction
- H_2/O_2 mechanism
- CO/O_2 mechanism
- CH_4 mechanism

NO_x Chemistry

- Three Mechanisms
  - Thermal
  - Prompt (includes fuel)
  - N_2O intermediate
- Regions of activity
- Zeldovich Mechanism (O_2, $N_2 \rightarrow$ NO)
  - Effects, limits: T, $[O]_{eq}$.
- Prompt: Fuel frag + $N_2 \rightarrow$ HCN $\rightarrow$ NO
- NO Control: combustion and post-combustion controls
  - NO vs T, NO vs ϕ, timescale
  - SCR, SNCR, explicity remove N_2 from feed (air separation, etc.)
- Quantities
  - Fuel NO_x = half of total
  - Limits: 15-40 ppmv