Chemical Engineering 633

Combustion Processes

Review 2

Exam 2 Review

- Classes 17-27
- Chapter 15
  - Pollutant Emissions
- Chapter 6
  - Canonical Reactors
  - Batch, PFR, PSR
- Chapter 7
  - Governing Equations
  - Shvab-Zeldovich
  - Conserved Scalars
- Chapter 8
  - Premixed Flames
  - Premixed Analysis
  - Flame Speed
  - Extinction/Ignition

•Reading: Chps 6-8, 15
•Homework assignments 5-6
•Class discussions

Pollutant Emissions

$$EI = \frac{m_i}{m_f} = \frac{x_i}{x_{co} + x_{co2}} \frac{n_c}{n_f} \frac{M_i}{M_f}$$

$$x_{dry} = \frac{x_{wet}}{1 - x_{h2o}} = x_{wet} \frac{N_{mix,wet}}{N_{mix,dry}}$$

- Emissions measures, CO, HC, SO_x
- Emission Index = mass emit / mass fuel
- Concentration (ppmv)
  - Dry or wet basis: convert between
  - Corrected concetrations (given O_2 basis)
- SO_x
  - From S in fuel: Coal, Diesel, (gasoline)
  - All S is converted to SO_x, unlike NO_x.
  - Limestone or lime scrubbing: $CaCO_3$, CaO → hydrated $CaSO_3$.
    - **Wet** or dry spray towers
- Ash/soot
  - Baghouse
- Unburnt HC/CO
  - Run lean, post combustion (3-way catalyst)
  - Engines: wall quenching/oil absorption.

Canonical Reactors

- Batch Reactor
  - Species balance (accumulation = source)
  - Write in terms of key quantities.
  - Versions: adiabatic, or given T; const P or const V.
    - Energy equation is optional depending on method.
- Plug flow reactor
  - Just a batch reactor with a time/space transformation with velocity.
    - Velocity given by $\dot{m}=\rho A v$

Reactors/Applications

- PSR
  - Algebraic equations: Inlet-outlet+generation = 0.
  - PSR residence time (tau = (rho*V/mdot))
    - Residence time “strains” the reactions like a diffusion or mixing term: reaction balances mixing.
  - Adiabatic, or isothermal.
  - Solve steady equations, or unsteady equations to SS (like Batch RXR)
  - Mixing term, Blowout
  - S-Curve
- Engine NO_x.
  - Model NO_x decrease during expansions stroke.
- Ignition Delay time for combustion.
- Chaining PFR reactors to simulate jet entrainment and contaminant species destruction.

Conservation Equations

- Coupling thermo, kinetics, and transport for generic systems, flames.
- Conservation Laws
  - Mass
  - Species
  - Momentum
  - Energy

$$\frac{dB}{dt} = \frac{d}{dt}\int_{CV} \rho b dV + \int_{A} \rho b \vec{v} \cdot \vec{n} dA$$

- Derive with Reynolds Transport Theorem
  - Lagrangian = Eulerian
  - Conservation law (CL) written for Lagrangian → CL = Eulerian
- Coordinate systems
  - Notes for gradient, divergence operator in Cartesian, Cylindrical, Spherical.
  - Notes for expanded mass and momentum equations from Bird et al.

Shvab-Zeldovich

- Simplify equations for analytic solution
  - SS
  - No P.E., K.E., Shaft work, viscous dissipation, heat sources (radiation).
  - Unity Le.

energy $$\rho\vec{v}\cdot\nabla h_s - \nabla\cdot\rho D\nabla h_s = -\sum_i h^o_{fi}\dot{m}_i'''$$

species $$\underbrace{\rho\vec{v}\cdot\nabla Y_i - \nabla\cdot\rho D\nabla Y_i}_{\textbf{transport}} = \underbrace{m_i'''}_{\textbf{source}}$$

  - Know the assumptions
  - Know the basic procedure (notes).
  - Axisymmetric simplifications

Conserved Scalars

- Under Shvab-Zeldovich assumptions, enthalpy is a conserved scalar
  - No source term
  - Known based on mixed state alone.
  - Knowing one conserved scalar gives all other conserved scalars.
- Mixture fraction transport equation.
  - Derive from definition of species transport equation, convert to elemental mass fractions, then mixture fraction.
  - No source term.
  - Great for modelling: can solve for mixture fraction and get other quantities (T, species) as functions of mixture fraction.
    - Equilibrium model: Y=Y(ξ), T=T(ξ)
    - Flamelet model: Flamelet equation derived in notes: Y=Y(χ,ξ), T=T(χ,ξ)

$$\frac{\chi}{2}\frac{d^2Y_i}{d\xi^2} = -\dot{m}_i'''/\rho \qquad \chi = 2D\left(\frac{d\xi}{dx}\right)^2$$

Premixed Flames

- Premixed flame intro
- General properties
  - flame speed
  - flame thickness
  - generally one stoichiometry
  - flame angle (can use to measure flame speed)
- Examples
  - Home furnaces/cooking ranges
  - Bunsen flames
  - Turbulent or laminar

Premixed Analysis

- "Simplified Analysis"
  - Derive flame speed and thickness relations
  - Shvab-Zeldovich energy equation
  - Zone **I**, Zone **II** (know properties/assumptions in each)
  - Energy balance in Zone **I**, Linear T profile in Zone 2
  - Use mass balance in Zone 2 for flame thickness relation
- Flame speed and thickness results
  - Know how to compute these
- Flame speed correlations

$$S_L \propto \sqrt{\frac{\alpha \dot{m}'''_F}{\rho_u}}$$

$$\delta \propto \frac{\alpha}{S_L}$$

Flame speeds

- Temperature dependence
  - Can infer from simplified analysis flame speed relation
  - Experimental → T_u^2 relation
- Pressure dependence
  - Can infer from simplified analysis flame speed relatio
  - Experimental → sqrt(T_u) relation, which is consistent with global methane kinetics.
- Equivalence ratio dependence
  - Mainly through the temperature dependence (peaks rich).
  - Speed drops and thickness increases off-stoichiometric
- Fuel dependence
  - Alkanes are similiar, slowly increasing speed with number of carbons
  - Ethylene then acetylene → fast increase
  - Hydrogen is speedy
- Stoichiometric methane at STP → ~ 0.5 m/s, 0.5 mm speed, thickness

Flammability / Ignition

- Quenching
  - Quenching distance
    - Balance heat release and heat transer: volumetric versus area.
    - Rearrange expression to write in terms of flame speed

$$d \propto \frac{\alpha}{S_L} \propto \delta$$

- Ignition radius follows from a similar analysis.
  - Ignition energy from the energy to heat up the mixture in the critical radius.