Chemical Engineering 140

Chemical Process Analysis
C.J. Radke
Tentative Schedule
Fall 2013

Week 0

*8/30 1. Definition of Chemical Engineering: flow sheet, reactor trains and separation processes, raw materials, power production and CO2 separation, Artemisinin production in e-coli bacteria.

Week 1

9/02 LABOR DAY

9/04 2. The chemical-engineering tool box, Conservation of mass: Overall (total) mass balance. Meaning of mass and molar densities

9/06 3. Unsteady filling of a tank with liquid: control volume and Matlab numerical solution of a 1st order ODE. Basis of RK algorithm, How to draw graphs, Definitions of unsteady state, steady state, and equilibrium

Week 2

9/09 4. Steady-state example (mixing in a tee), Unsteady filling of a tank with an ideal gas: constant control volume.

9/11 5. Unsteady species balance with no chemical reaction: species balances (# of independent species balances). Washout of salt from a tank: dilute solutions, Meaning of residence time.

9/13 6. Unsteady species balance with chemical reaction: well-mixed, homogeneous reactions, Meaning of reaction rate, Steady state CSTR with 1st order irreversible kinetics,

Week 3

9/16 7. Definition of conversion. Controlling conversion by residence time, Comparison of conversion between a BSTR and a CSTR. Start-up of a CSTR with 1st order irreversible kinetics. Approach to steady state. Definition of residence time vs reaction time constants

9/18 8. Mathematical solution of ODEs: Characterization, General integrating factor solution for 1st order ODEs, Summary chart of equation types. Illustration of Matlab for nonlinear ODEs.

9/20 9. Steady mass balances. Species balances at steady-state with no chemical reaction: Basis selection. Simultaneous linear equations, Solution by Matlab. Degrees of freedom.

Week 4

*9/23 10. Multiple units: two distillation columns, Lack of independence of control volumes, Definition and use of tie components. DoF Analysis, Steady element balances with chemical reaction

9/25 11. Combustion of heptane. Degree of freedom analysis, Excess air, Element balances, Solution for systems of algebraic, equations using Matlab.

9/27 12. Reaction stoichiometry and conversion, Application of conversion to combustion of heptane, Stoichiometry and extent of reaction, Application of extent of reaction to combustion of heptane

Week 5

9/30 13. Production of rutile from Sorel slag

10/02 14. Review of the tool box. Chemical reaction equilibria: The ultimate conversion, Criterion for reaction equilibria: chemical potential change upon reaction. Equilibrium constants: The missing one! Comments on the methanol economy.

10/02 MIDTERM #1

10/04 15. Methanol from syngas, Equilibrium constants to obtain ultimate conversion: Use of conversion, extent of reaction, and element balance. Solution of single nonlinear algebraic equations by Succesive Substitution and Newton-Raphson iteration: application to methanol synthesis.

Week 6

10/07 16. Effect of pressure on equilibrium conversion, LeChatelier's principle for role of P. Effect of temperature on K and equilibrium conversion. Endothermic vs. exothermic reactions, Calculation of K from standard heats of reaction. LeChatelier's principle for role of T on equilibrium conversion

10/09 17. Ammonia synthesis. Importance of fertilizers in world food production. Design of an ammonia synthesis gas plant. An ammonia synthesis gas plant, steam reforming, water-gas shift rxn, burn out of oxygen, inerts that are in air, Plug flow (or packed-bed) reactor. What is a catalyst?

10/11 18. Equilibrium constraints on ammonia PFR reactor operating conditions: Need for high pressure and low temperature. Ammonia synthesis: condenser, recycle, and purge, Mass balance on Haber process.

Week 7

10/14 19. Ammonia synthesis: recycle ratio, overall conversion vs. single-pass conversion, single and multipass heat exchangers

10/16 20. Schematic of Haber-Bosch process. Design of ammonia reactor: species balances on a PFR.

10/18 21. Incorporation of realistic kinetics into design equation, Application of Runge-Kutta numerical solution of PFR design equation (Matlab). Scaling to a production-size reactor

Week 8

10/21 22. Effect of temperature on ammonia reactor size and conversion, LeChatelier vs. Arrhenius in ammonia-reactor design. Heat transfer in ammonia reactor. Actual reactor configuration. Pressure-Volume-Temperature properties for pure fluids: isothermal compression/expansion of an ideal gas. Lennard-Jones interactions

10/23 23. van der Waals equation of state and its physical origin. Isothermal compression/expansion of a real gas, Gas/liquid phase transition: dew points, bubble points, binodal, spinodal. Definition and meaning of quality in the two-phase region.

10/25 24. Fluid phase equilibrium: equality of chemical potential, Why do liquids (and solids) form? Vapor pressure, Antoine's equation. Pressure-temperature diagrams, Critical point, Law of corresponding states.

Week 9

10/28 25. Gibbs phase rule. Steam tables, superheated steam, saturated steam, compressed liquid, Finding properties in Regions I-III of steam tables. Real fluids: The complete phase diagram. Location of triple point and critical points, solid/vapor and solid/liquid equilibria.

10/30 26. Multicomponent L/V phase equilibria, Ideal gas and ideal liquid mixtures, Raoult's law, Setting the temperature of the ammonia condenser by Raoult. K factors for nonideal mixtures

11/01 27. Flash/condenser calculations by Newton iteration. Equilibrium ammonia-condenser design

Week 10

*11/04 28. Limits on flash/condensation conditions: multicomponent bubble and dew points. Water/air phase equilibria, air saturated with water vapor

*11/06 29. Partial water saturation in air, Relative humidity, Humidity, Liquid/liquid phase equilibria, Nernst partition coefficient, Extraction

11/06 MIDTERM # 2

*11/08 30. Distribution/partition coefficient, Extraction equilibrium, Concepts in separation processes: Equilibrium stages and mixers/settlers, Concept of equilibrium stage, Mass transfer flux, characteristic time

Week 11

11/11 VETERAN'S DAY

11/13 31. Equilibrium Concepts in Separation Processes cont: Multistaging, cross, co, counter current flow, Kremser equation, Distillation and extraction towers

11/13 Writing skills (voluntary)

11/15 32. Energy conservation: forms of energy: internal energy. State functions , Definition of work and power. Path vs state functions, Reversible work, PV work in expansion of a piston. Heat transfer flux, Definition of overall and individual heat transfer coefficients,

Week 12

11/18 33. Concept of heat transfer resistance by analogy to Ohm's law, Heat transfer resistances in series, General unsteady energy balance, Flow work vs shaft work, Introduction of enthalpy

11/20 34. Unsteady closed form (the "First Law"), Steady open form of general energy balance ("Enthalpy Balance"). Steady mixing of hot and cold fluids in a tee

11/22 35. Transient steam heating of liquid in a CST, Characteristic time. Steady steam tracing of a liquid in a CST. Steam exit quality.

Week 13

11/25 36. Enthalpy balances with chemical reaction.

11/27 No class

11/29 THANKSGIVING

Week 14

12/02 37. Standard heats of reaction. Steam reforming of methane

+12/02 38. Evaluation of sensible and latent enthalpy changes, Adiabatic flame temperature (Thanksgiving makeup lecture)

*12/04 39. Production of calcium oxide from limestone: Charting steady enthalpy balances.

12/06 40. Design of double pipe heat exchanger

Week 15

12/09 41. Review, Course evaluation forms.

FINAL EXAMINATION

12/16 Monday, December 16, 7-10 p

* indicates instructor's absence
+ indicates makeup lecture