Chemical and Biomolecular Engineering 140
Introduction to Chemical Processes
Spring Semester 2021

Objective: To introduce the principles of mass and energy balances with equilibrium and rate expressions for solving basic chemical engineering/science problems.

Text: Required:
Felder and Rousseau, “Elementary Principles of Chemical Processes,” 3rd ed., John Wiley and Sons (2005).

Recommended:
1. Murphy, “Introduction to Chemical Processes,” McGraw-Hill (2007).
2. Himmelblau and Riggs, “Basic Principles and Calculations in Chemical Engineering,” 8th ed. Prentice-Hall (2012).
3. Duncan and Reimer, “Chemical Engineering Design and Analysis: An Introduction,” Cambridge University Press (1998).
4. Russell and Denn, “Introduction to Chemical Engineering Analysis,” John Wiley and Sons (1972).
5. Shreve, “The Chemical Process Industries,” McGraw-Hill (1956).

Description: CBE 140 presents analysis of chemical processes. Such an analysis depends on the ability to construct balances on mass and energy within a system. This course is basic to what follows in the curriculum in terms of transport phenomena (150A&B), thermodynamics (141) and kinetics (142). In other words, this is really a base course of the chemical engineering curriculum. The required text is followed very loosely, i.e., lecture material will not necessarily follow the text. Students are encouraged to refer to other recommended texts when necessary.

COURSE SCHEDULE

Total Lectures: 40

Week 1:

January 20
Overview of Chemical Engineering Discipline: *flow sheets, reactor trains, separation processes and raw materials,*
Conservation of Mass,
Overall (total) unsteady mass balance and meaning of mass densities

January 22
Unsteady tank filling with a liquid,
Classification of ODEs,
Definitions of unsteady state, state state and equilibrium,
Steady-state examples: Steady mixing in a tee

Week 2:

January 25	Meaning and choice of Control Volumes (CVs) Unsteady filling of a tank with an ideal gas: constant Control Volume,
January 27	Problem solving, reading and schematics, Process flow diagram for propene production, Unsteady species balance with no chemical reaction: *species balances and (number of independent species balances)* Washout of salt from a tank: dilute solution, meaning of residence time
January 29	General species balance with chemical reaction, Importance of using moles, Meaning of homogeneous reaction rate, Kinetic rate expressions Types of well-mixed reactors, Steady CSTR with 1^{st} order, irreversible kinetics, Definition of Conversion

Week 3:

February 1	Review of CSTR, Transient BSTR with 1^{st} order irreversible kinetics, Conversion in an unsteady BSTR and comparing conversions in the two reactors Start-up of a CSTR with 1^{st} order irreversible kinetics, Approach to steady state, residence times vs. reaction time constants
February 3	Transient BSTR with multiple reacting species, Reaction rates and stoichiometry, Number of independent equations
February 5	Steady species balances with no chemical reaction, basis selection, Degrees of freedom, Multiple units: *two distillation columns, lack of independence, Definition and use of tie components,* DoF Analysis.

Week 4:

February 8	Steady mole balance with reaction by element balances, Combustion of heptane DoF Analysis: Basis, Excess air, No CO or heptane in product
February 10	Combustion of heptane (continuation) Steady mole balance with reaction by conversion, Steady mole balance with reaction by extent of reaction, Extent of reaction for multiple reactions and comparison of approaches

February 12	Process Analysis with reaction and multiple equipment: *Production of Rutile from Sorel Slag*

Week 5:

February 15	Holiday
February 17	Chemical reaction equilibria: *The ultimate conversion, and criterion for reaction equilibria* Chemical potential for ideal gas mixture: *Boltzmann expression for entropy*.
February 19	Equilibrium constants, the missing one. Methanol economy: Methanol from syngas Equilibrium constant to obtain ultimate conversion: *Use of conversion* Use of extent of reaction in reaction equilibria

Week 6:

February 22	***MIDTERM: Mid term 3:00p-4:00p, Monday (During lecture on zoom)***
February 22	Use of element balances in reaction equilibria Comment on degree of freedom analysis, Effect of pressure on equilibrium conversion, Le Chatelier's principle for role of P
February 24	Effect of temperature on K and equilibrium conversion, Endothermic vs. exothermic reactions and bond energies Calculation of K from standard heats of reaction Le Chatelier's principle for role of T Ammonia synthesis and gas plant
February 26	Plug Flow Reactors (PFR) Catalysts Equilibrium constraints on ammonia PFR reactor operating conditions: *Need for high pressure and low temperature*

Week 7:

March 1	Design of ammonia reactor: *species balances on a PFR* PFR design equation, Incorporating realistic kinetics
March 4	Numerical solution of PFR design equation, Scaling to a production-size reactor, Effect of temperature on ammonia reactor size and conversion Le Chatelier vs. Arrhenius in ammonia reactor design

March 5 — Hot spot in ammonia reactor, Actual reactor configuration
Incorporating reactor design in ammonia synthesis
Reactor, Condenser, Recycle and Purge
Mass balance on Haber process

<u>Week 8:</u>

March 8	Mass balance on Haber process: *Recycle ratio, overall conversion vs. single-pass conversion* Heat management in ammonia synthesis (Heat flux and temp. difference) Newton's law of heating/cooling, Co-current, counter-current and cross flow, single and multiple heat exchangers
March 10	Pressure-Volume-Temperature (PVT) properties for fluids, Isothermal compression/expansion of ideal gases, Lennard-Jones interactions and origin of van der Waals EOS, Isothermal compression/expansion of real gas, Gas/liquid phase transitions (dew points, bubble points & vapor pressure)
March 12	Definition and meaning of quality in the two-phase region, Fluid phase equilibria: *equality of chemical potential*, Vapor pressure as function of temperature, Antoine's equation

<u>Week 9:</u>

March 15	Real fluids, P-T diagrams, Critical point, Law of corresponding states from VdW EOS, 3 parameter corresponding states, Kay's rule for mixtures Steam tables, superheated steam, saturated steam, subcooled liquid
March 17	The complete phase diagram: Location of triple & critical points Solid/vapor and solid/liquid equilibria (pure fluids), Gibbs phase rule
March 19	Multicomponent liquid/vapor phase equilibria Ideal gas & Ideal liquid mixtures, Raoult's law, K factors for nonideal mixtures, Analogy to reaction equilibrium constants

<u>Week 10:</u>

March 22	Spring Recess
March 24	Spring Recess
March 26	Spring Recess

Week 11:

March 29	Flash/condenser calculations, effects of multicomponent bubble and dew points Equilibrium ammonia-condenser design in Haber process
March 31	Liquid/liquid phase equilibria Nernst partition coefficient, Distribution/partition coefficient, Extraction equilibrium Concepts in separation processes
April 2	Mass transfer flux Criterion for equilibrium stage: *ratio of characteristic time for mass transfer relative to residence time* Single-stage extraction with Nernst law for separating ethanol from water by dodecanol in a single stage

Week 12:

April 5	Proctor and Gamble: Loss of liquid-soap fragrance in showering
April 5	***MIDTERM: Mid term 3:00 – 4:00p, Monday (In Lecture hour on zoom)***
April 7	Multistaging: cross, co, counter-current flow with two stages, Counter-current extraction with N equilibrium stages
April 9	Kremser equation for N counter-current equilibrium stages Energy conservation: *Different forms of energy, State functions*

Week 13:

April 12	Work and power, Path vs. state functions, Reversible work, PV Work Definition of Heat, Heat transfer coefficient, Heat transfer resistance Unsteady energy balance, flow work vs. shaft work, enthalpy
April 14	Enthalpy as a state property, Unsteady closed form of energy balance Steady open form of general energy balance
April 16	Closed system examples: *Freezing of liquid water in a container, adiabatic and isothermal chemical reactions, enthalpy of reactions in energy balance*

Week 14:

April 19	Steady open system example: steady mixing of hot and cold fluids in a tee Transient steam heating of liquid in a CST

April 21	Transient steam heating of liquid in a CST (continued) & Characteristic time Steady steam tracing of liquid in a CST & steam exit quality
April 23	Steady enthalpy balances with chemical reaction Standard heats of reaction Enthalpy balances with reaction including latent heats

<u>Week 15:</u>

April 26	Steam reforming of methane, Mean heat capacities, Hess's law for standard heats of reaction
April 28	Adiabatic flame temperature, Production of calcium oxide from limestone: *Couple mass and energy balances for multiple reactions*
April 30	Charting steady enthalpy balances Comparison to enthalpy balance using multiple extents of reaction
<u>Week 16:</u>	RRR Week

FINAL EXAMINATION:

May :	To be updated