Chemical Rxn Engineering CHE06316-02 Schedule of Topics for Spring 2017

Polymath: Nonlinear Equation Solver (NLE)

Polymath: Differential Equation Solver (DEQ) & COMSOL

**ASPEN**

Polymath: Regression

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| **Date:** | **Proposed Topics for 4 Credit Hour Class** Monday & Wednesday 9:30 AM-10:45PM (ROW 340),  Friday: 11:00 - 1:45PM (ROW 340), **Double Period**  **This is a tentative list of topics that will be updated under Schedule of Topics in Blackboard** |
| **January** 18 Wednesday | An Introduction to Reactor Design: What do you need to know?  Overview of Reactors and Reactor Design: **Chapter 1**, 1.5 Industrial ReactorsReview of Stoichiometry: **Chapter 2 and 4** 2.1-2.2 Definition of Conversion, χ 4.1-4.2 Stoichiometric Table **for batch and flow systems  Windows Laptops: Install ASPEN before 1/20/17; Apple computers use cloud** |
| 20 Friday | **PCP II Review Dehydrogenation of Ethylbenzene: Stoic Tables and Energy Balances**  Fogler’s Text and CD-ROM Introduction to Semester Design Projects  **Memo 1: Overall Balances Assigned** **Computer Laboratory: ASPEN 1 – Stoichiometric Reactors** |
| 23 Monday | **Chapter 1: Mole Balances:  1.1 - 1.3** Accumulation = in - out + generation. – Batch, Semi-Batch  1.4.1 Mole Balances cont*:*  Accumulation = in - out + generation. **–** CSTR |
| 25 Wednesday | 1.4.2 & 1.4.2 Mole Balances cont*:*  Accumulation = in - out + generation. **–** PFR and PBR **Chapter 6:** Why use χ when you can use *CA* and *FA*? **Batch Reactors** 2.1-2.2 *V* = f(χA, *rA*)  2.6 definitions of space time, space velocity, and residence time |
| 27 Friday | **Chapter 2 Conversion and Reactor Sizing:  Flow Reactors** 2.3- 2.5 Graphical representation of *V,* reactors in series and parallel; Cutlip and Shacham Problem 3.13 k=f(T) |
| 30 Monday | **Chapter 3 Rate Laws and Stoichiometry** 3.1 & 3.2 Rate Laws and order of reactions3.2.1 & 3.2.2 Elementary reactions, Non-elementary reactions (LHHW example) 3.2.3 Rate expressions for reversible reactions & equilibrium  3.3 Arrhenius reaction rate "constant”4.2.3 Gas expansion in tubular reactors (PFR’s) Polymath Model Cutlip and Shacham Problems 11.1 & 11.2 **Due: Reactor Design Memo 1: Overall Balances** |
| **February**  1 Wednesday | 4.2.3 Gas expansion in tubular reactors (PFR’s) Conversion Model  **Chapter 5 Isothermal Reactor Design** "Plug in *rA* = f(χA, *CA,* *CB*, ...) into mole balance"  5.4 Isothermal Reactor Design – Tubular Reactors "Plug in *rA* = f(χA, *CA,* *CB*, ...) into mole balance" |
| 3 Friday | **Computer Laboratory – ASPEN 2 – Power Law Rate Expressions** |
| 6 Monday | 5.5 Pressure Drop in Reactors: Packed beds: constant gas density & variable gas densitySee example 5-5 for effect of particle size on pressure drop and conversion  Cutlip and Shacham Problems 11.3 |
| 8 Wednesday | Example Problem of Packed Bed Reactor: o-Creosol to 2-methylcyclohexanone |
| 10 Friday | 5.2 Batch Reactors5.3 Isothermal Reactor Design - CSTR "Plug in *rA* = f(χA, *CA,* *CB*, ...) into mole balance" 5.3.2 CSTR in Series (Tanks in Series Model) Cutlip and Shacham Problem CSTR in Series 11.6 5.6 (Read) Synthesizing a Chemical Plant  **Due: Reactor Design Memo 2: Reactor volume using simple reaction rate expression** |
| 13 Monday | 6.3 Molar Flow Rate Algorithm to Microreactors6.4 Membrane Reactors  Cutlip and Shacham Problem 11.4 Catalytic Membrane Reactor(8.4 1st ed.) *Green Engineering: Pollution Prevention Applications for Separative Reactors* |
| 15 Wednesday | 6.5 Unsteady-state analysis: 13.4 Unsteady-state CSTR and 6.6 Semibatch reactors  Cutlip and Shacham Problem 8.5 Semibatch |
| 17 Friday | Review for Exam1  **Design Consultations**  **Computer Laboratory – ASPEN 3 –Pressure Drop in Fixed Bed Reactors** |
| 20 Monday | **Cancelled** |
| 22 Wednesday | **Cancelled** |
| **24 Friday** | **Chapter 11 Nonisothermal Reactor Design – Adiabatic Operation of a PFR**  *Green Engineering: Minimizing Energy Consumption Related to Reactors* 11.2 Review of energy balances: Nonisothermal continuous-flow reactors at steady-state Overview of Energy Balances for CSTR, PFR, & Batch  **Exam 1 – Chapters 1-5.4 (for simple reactions) (no pressure drop on exam 1)**  **Due: Reactor Design Memo 3: Pressure Drop** |
| 27 Monday | 11.4 Adding the energy balance to the PFR equations - adiabatic**.** Appendix C: Review of the prediction of the equilibrium constant See also Example 3-6: Calculating the Equilibrium Conversion  11.5 Equilibrium Conversion (χeq with energy balances) 11.6 Reactor Staging 11.7 Optimum Feed Temperature  Cutlip and Shacham Problems 11.22 Batch, 11.23 CSTR, 11.24 PFR, 11.25 PFR&CSTR |
| **March** 1 Wednesday | **Chapter 8 Multiple Reactions** 8.3 Selectivity in Parallel8.4 Selectivity in Series Reactions 8.5 Complex Reaction Networks Cutlip and Shacham Problem 11.21 (8.21 1st ed.) *Aspects of Green Engineering Related to Selectivity* |
| 3 Friday | **Computer Laboratory ASPEN 4: Multiple Reactions** |
| 6 Monday | Chapter 12: 12.1 Steady-State Tubular Reactor with Heat Exchange  12.2 Balance on the Heat-Transfer Fluid 12.3 Adding the energy balance to the PFR equations – adiabatic |
| 8 Wednesday | 12.4 CSTR with Heat Effects  12.6 Energy Balances for Multiple Reactions |
| 10 Friday | 12.5 Multiple steady-states  Cutlip & Shacham 6.3 multiple steady states with ODE’s |
| March 13-17 | **SPRING BREAK** |
| 20 Monday | **Project Day** |
| 22 Wednesday | **Chapter 7 Collection and Analysis of Rate Data** Batch reactors 7.2 Method of Excess  7.4 Differential method 7.3 Integral method7.5 Least Squares Analysis 7.1 Initial rates method 7.6 Differential reactors  (Read) Laboratory reactors in notes  Cutlip and Shacham Problems 3.10 – 3.13 & 11.7 – 11.15 (1st ed. 2.10 – 2.13, 8.7-8.15) |
| 24 Friday | 7.3 Integral method7.5 Least Squares Analysis 7.1 Initial rates method 7.6 Differential reactors  (Read) Laboratory reactors in notes  **Chapter 10 Catalysis and Catalytic Reactors** 10.1 Catalysts  10.2 Mechanisms of catalytic reactions: Langmuir-Hinshelwood Rate Expressions, Use of Charts –Langmuir-Hinshelwood Rate Expressions originally from Yang, K.H. and Hougen, O.H. Chem. Eng. Prog. 46 146 (1950). 10.2.2 Surface reactions Generalized expression for *rA* for heterogeneous catalysis  10.2.4 rate limiting step  **Due: Reactor Design Memo 4: Multiple Reactions** |
| 27 Monday | 10.4 Heterogeneous Data Analysis for Reactor Design ***Green Engineering – Choice of Catalysts to minimize generation of unwanted chemicals*** |
| 29 Wednesday | 10.7 Catalyst DeactivationCutlipand Shacham Problems 3.10, 3.11, 3.12, 8.18 & 8.19 |
| 31 Friday | **Chapter 9 Bioreactors Design Consultations** |
| **April** 3 Monday | **Chapter 13 Unsteady-State Nonisothermal Reactor Design** 13.2 Energy Balance on Batch Reactors Safety Presentation: Batch Styrene Polymerization Reactor Runaway – SACHE **Example 13-6 T2 Laboratories Explosion** |
| 5 Wednesday | **Chapter 14 Mass Transfer Limitations in Reacting Systems** 14.4 Mass transfer limited reactions and surface reaction limited reactions  14.4.3 Mass Transfer-Limited Reactions in Packed Beds **Exam 2 Review** |
| 7 Friday | **Computer Laboratory – COMSOL 1**  **EXAM 2: Chapters 5.5, 6, 8, 11 &12** |
| 10 Monday | **Chapter 15 Diffusion and Reaction in Porous Catalysts** 15.2 Mole balance in a porous catalyst particle 15.3 Internal Effectiveness Factor Cutlip and Shacham Problems 6.5 Diff&rxn, 10.5η, 10.6η, 10.7 Diff&rxn, 10.11 Diff&rxn, 10.12η,  10.14 Diff&rxn,10.15 Diff&rxn |
| 12 Wednesday | 15.4 Falsified kinetics 15.5 Overall Effectiveness Factor 15.7 Mass Transfer and Reaction in a Packed Bed  **Due: Reactor Design Memo 5: Energy Balance for Multiple Reactions** |
| **14 Friday** | **Good Friday: No Classes** |
| 17 Monday | **Industrial Mixing in Chemical Reactors**  **Chapter 16: Residence Time Distributions and Chapter 17: Mixing in Reactors** Experimental Observations of RTD’s  14.4 Dispersion in Tubular Reactors in Turbulent and Laminar Flows |
| 29 Wednesday | **Chapter 18: Models for Nonideal Reactors** |
| 21 Friday | **Chapter 18 Continued** |
| 24 Monday | Project Week |
| 26 Wednesday | Project Week |
| 28 Friday | **Project Presentations  Due: Reactor Design Final Report** |
| **May** 1 Monday | Review for Final Exam |
| May 3 | Comprehensive Final  10:15 AM - 12:15 PM Rowan Hall 340 |
|  | Go out and design some reactors! |