ChemE 3900 - Chemical Kinetics & Reactor Design - Spring 2021
Part 2 - Reactor Analysis & Design

	date	topics	reading
R1	Mon 3/22	Reactor Design and Analysis. Introduction & overview. Reactor parameters & their limits. Reactor types. Applications, advantages, and disadvantages of each.	Levenspiel: Chp. 4. Hill & Root: Chp 8, pp. 216-225.
R2	Wed 3/24	Performance/design equations for batch reactors, CSTRs and plug flow reactors. Fractional conversion, residence time, and Levenspiel plots.	Levenspiel: **5.1**, **5.2**. Hill & Root: Chp 8, pp. 225-228.
R3	Fri 3/26	Example calculation for a batch reactor. Limiting reactant. Daily production. Graphical method for maximum daily production.	Levenspiel: **5.3**
R4	Mon 3/29	Comparison of a single CSTR and a single PFR. Reactor volume and fractional conversion. Multiple PFRs in series.	Levenspiel: **6.1, 6.2** Hill & Root: Chp 8, pp. 228-240.
R5	Wed 3/31	Multiple CSTRs in series. Mathematical analysis with design/ performance equations and graphical analysis with design/ performance maps.	Levenspiel: **6.2** Hill & Root: Chp 8, pp. 241-253.
R6	Fri 4/2	Reactor design for an autocatalytic reaction. A plug flow reactor with a splitter recycle.	Levenspiel: **6.3, 6.4** Hill & Root: Chp 8, pp. 253-254.
R7	Mon 4/5	Reactor design for multiple reactions - example reactions and reactor variations. Reactions in parallel. Fractional yield - instantaneous (differential) and total (integrated).	Levenspiel: Chp. 7, pp. 152-160. Hill & Root: Chp 9, pp. 273-278.
R8	Wed 4/7	Reactor design for reactions in parallel, cont'd. Graphical analysis with φ vs. [A]. The Trambouze Reactions.	Levenspiel: Chp. 7, pp. 161-164.
R9	Fri 4/9	Reactor design for reactions in parallel, cont'd. Selectivity - instantaneous (differential) and total (integrated). Reactor design for reactions in series. Concentrations as a function of τ for PFRs.	Levenspiel: Chp. 8, pp 170-180. Hill & Root: Chp 9, p. 278-282.
R10	Mon 4/12	Reactor design for reactions in series, cont'd. Concentrations as a function of τ for CSTRs. Fractional yield vs. [A] for PFRs and CSTRs.	Levenspiel: Chp. 8, pp 181-185.
R11	Wed 4/14	Reversible reactions - single reaction, reactions in series and reactions in parallel. Reaction trajectories on ternary diagrams. Reactor design for series-parallel reactions - two-step irreversible reaction. Analytical and graphical analysis.	Levenspiel: Chp. 8, pp 185-200. Hill & Root: Chp 9, pp. 287-289.
R12	Fri 4/16	Reactor design for series-parallel reactions, cont'd. Graphical analysis examples. How to calculate residence times.	
R13	Mon 4/19	Thermodynamics of chemical reactions. Criteria for spontaneous reaction and equilibrium. Reaction quotient & equilibrium constant as a function of fractional conversion. Effect of pressure on composition at equilibrium. Effect of temperature on equilibrium constant - Gibbs-Helmholtz and van't Hoff equations.	McQuarrie & Simon: **26.1-26.7**. Levenspiel: Chp. 9, pp 207-215. Hill & Root: Chp 2, pp. 4-15.
R14	Wed 4/21	Thermodynamics of chemical reactions. Heat removed from an isothermal reactor. Temperature change in an adiabatic reactor. Levenspiel plots for adiabatic reaction as a function of activation energy. Batch times as a function of conversion in an adiabatic reactor; conversion for maximum production rate.	Hill & Root: Chp 10, pp. 305-317.

	Fri 4/23	*No lecture – Wellness Day.*	
	Mon 4/26	*No lecture – Wellness Day.*	
R15	Wed 4/28	Temperature programs for batch reactors. Reaction rate contour lines on temperature-conversion maps.	Levenspiel: Chp. 9, pp 215-223.
R16	Fri 4/30	Temperature programs for batch reactors, cont'd. Reaction trajectories for adiabatic and isothermal operation. Translating a reaction trajectory to a Levenspiel plot. Temperature programs for flow reactors. Series plug flow reactors with interstage cooling/heating. Optimal trajectory to a target conversion.	Levenspiel: Chp. 9, pp 223-226.
R17	Mon 5/3	Temperature programs for flow reactors, cont'd - CSTRs. Analysis of adiabatic CSTRs on temperature-conversion maps. Levenspiel plots for adiabatic CSTRs.	
R18	Wed 5/5	Analysis of adiabatic CSTRs, cont'd. Multiple steady states in CSTRs - ignition and extinction temperature, stable and unstable operating conditions. PFRs with recycle cooling.	Levenspiel: Chp. 9, pp 226- 235, Chp 19, pp. 427-443. Hill & Root: Chp 10, pp. 320-324.
R19	Fri 5/7	Non-isothermal flow reactors. CSTR vs. PFR vs. PFR with recycle - relative advantages. Temperature program strategies for series-parallel reactions. Strategies for constrained design and/or operation.	Levenspiel: Chp. 10. Hill & Root: Chp 10, p. 324-327..
R20	Mon 5/10	Reactor design for solid catalysts. Survey of reactor configurations. Overview of principal rate processes - length scales and elementary transport steps in porous catalysts. Diffusive mass transfer across film external to catalyst pellet.	Levenspiel: Chp. 17; Chp. 18, pp. 376-391. Hill & Root: Chp 6, pp. 160-163.
R21	Wed 5/12	Reactor design for solid catalysts, cont'd. Definitions of catalytic reaction rates: homogeneous rate, surface reaction rate, and catalyst mass rate. Porous catalyst particles - mass transfer and chemical reaction in a single pore - the effectiveness factor, η, the Thiele modulus and the Damköhler group II. Analysis for spherical porous catalyst pellets.	Hill & Root: Chp 12, pp. 371-394.
R22	Fri 5/14	Analysis for spherical porous catalyst pellets, cont'd. Example exercises in reactor design and performance for solid catalysts.	
		Principles of kinetics applied to non-chemical systems; the social kinetics of slope day.	

References:

O. Levenspiel, *Chemical Reaction Engineering*, 3rd ed. (Wiley, 1999)

C. G. Hill and T. W. Root: *Introduction to Chemical Engineering Kinetics & Reactor Design*, 2nd ed. (Wiley, 2014).

McQuarrie & Simon, *Physical Chemistry - A Molecular Approach* (University Science Books, 1997)