CHEE 420/520
Chemical Reaction Engineering
Department of Chemical and Environmental Engineering
Fall 2015
The University of Arizona
T/Th, 9:30 – 10:45 AM; Harvill, Room 204
Syllabus (*The information contained in this syllabus is subject to change)*

Instructor: Prof. Armin Sorooshian (armin@email.arizona.edu)
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Teaching Assistant: Mojtaba Azadi Aghdam (mojtabaa@email.arizona.edu)
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Preceptor: Taylor Shingler (taylors@email.arizona.edu)
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Office Hours: Mon 1-3

(Email all technical HW questions to Mojtaba and Taylor)
(Email all grading-related HW questions to Zhen Wang: zhenw@email.arizona.edu)

Prerequisites: CHEE 201, CHEE 326, MATH 254

Course Website: D2L website for ChEE 420/520
Textbook: Elements of Chemical Reaction Engineering, H. Scott Fogler, 4th ed. (2006)

Course Objective: Study and apply the fundamental principles of chemical reaction engineering to design and analyze basic chemical reactors that contain both homogeneous and heterogeneous reactions.

Lecture Topics (Chapters 1-8, 10-12)
- Chemical Kinetics
- Isothermal and Nonisothermal Reactor Design
- Catalysis

Grading Scheme:

A (100 - 90%)	B (89 - 80%)	C (79 - 70%)	D (69 - 60%)	E (< 60%)

Problem Sets	10%
Exam 1	20%
Exam 2	20%
Exam 3	20%
Final Exam (Tuesday December 15, 2015, 08:00-10:00)	30%

HW: Homework is due at the beginning of class on the scheduled due date. To receive credit, all work must be original and that of the student and not from any other source (e.g. other students, solution manuals, etc). Late homework will not be graded. Homework that is not stapled or that does not have your name will not be graded and will receive a grade of 0%. Students have 1 week from the day that HW or exams are returned to discuss grading issues. All work that is not picked up beyond 1 week after the first day a return is attempted will be recycled to ensure students are responsible and up-to-date. Graded HW can be picked up outside the instructor's office in the hallway as soon as you see grades uploaded onto D2L.

Exams: There will be four exams, each of which will be cumulative. Exams are open book, and 75 minutes long (final exam though is two hours). You can use calculators and pencils (all other materials you will need for the exam will be provided). No hats or anything that beeps. If you sit next to regular study partners and those you normally sit by in class, you will receive a grade deduction.

Make-up exams: A make-up exam may be arranged if you notify the instructor before the regularly-scheduled exam. A makeup exam will be scheduled only if the student has a valid reason for missing the regularly scheduled exam.

Students with Special Needs: It is the University's goal that learning experiences be as accessible as possible. If you anticipate or experience physical or academic barriers based on disability or pregnancy, please let me know immediately so that we can discuss options. You are also welcome to contact Disability Resources (520-621-3268) to establish reasonable accommodations.

Standards for Presentation of Results in HW and Exams:

- For more details, see the very end of the syllabus
- Restate problem statements with a sketch when appropriate with proper labeling of given values and quantities looked up.
- In order to expedite the grading process, clearly show the main steps in your analysis and put circles/boxes around the key values and the final answer.
- Report units at important intermediate stages and in the final answer.
- Indicate the basis you select, and indicate any change of basis within the problem. State assumptions.
- Values obtained from a handbook or other reference should be accompanied by a citation to the source (i.e. text and page number).
- Use 8.5 x 11 inch paper. Multiple pages must be stapled together. First page should have the student's full name, the course number, problem set #, and date the assignment was turned in. All following pages should have student's last name and page number (example: Sorooshian, 2).
- Complete problems sequentially, so that arrows are not required to guide grader to next part of problem. Write legibly and neatly; using the back of pages is encouraged unless using a pen that "bleeds" through the page.

Classroom policy: Turn off all things that beep (e.g. phones, ipods, pagers)
Code of student conduct: http://deanofstudents.arizona.edu/studentcodeofconduct
Code of academic integrity: http://deanofstudents.arizona.edu/codeofacademicintegrity
Policy on threatening behavior by students: http://policy.web.arizona.edu/~policy/threatening.pdf

CHEE 420/520 – Class Sequence – Fall 2015:

Date			Topic	Reading	Important Events
Aug	T	25	Syllabus/Introduction; Material Balances for Reactors; Conversion	1.1-1.5, 2.1-2.3, 4.1-4.4	
	Th	27	Continue: Material Balances for Reactors & Conversion	1.1-1.5, 2.1-2.6, 4.1-4.4	
Sep	T	1	Review of Thermo/Kinetics; Graphical Representation of Design Equations	1.1, 3.1-3.6, 2.1-2.6, 4.1-4.4	
	Th	3	Continue: Graphical Representation of Design Equations; Design of Isothermal Reactors (N^{th} Order Kinetics)	2.1-2.6, 4.1-4.4	HW 1 Due
	T	8	Reactors in Series and Introduction to Pharmacokinetics	2.1-2.6, 4.1-4.4	
	Th	10	Continue: Reactors in Series/Parallel	2.1-2.6, 4.1-4.4	HW 2 Due
	T	15	Pressure Drops in Reactors	4.5	
	Th	17	Continue: Pressure Drops in Reactors	4.5	
	T	22	Unsteady Operation of CSTRs/semi-batch reactors; Data Analysis in Reactors	4.10, 5.1-5.7	HW 3 Due
	Th	24	Continue: Data Analysis in Reactors	5.1-5.7	
	T	29	Multiple Reactions	6	
Oct	Th	1	Continue: Multiple Reactions; Review	6	
	T	6	Exam 1		Exam 1
	Th	8	Review Exam 1; Continue: Multiple Reactions	6	HW 4 Due
	T	13	Continue: Multiple Reactions	6	
	Th	15	Reaction Mechanisms	7.1	
	T	20	(Sub Teacher) Continue: Reaction Mechanisms	7.2 - 7.3	
	Th	22	(Sub Teacher) Continue: Reaction Mechanisms (Enzymes)	7.2 - 7.3	HW 5 Due
	T	27	Continue: Reaction Mechanisms (Enzymes); Steady State Non-Isothermal Reactor Design	7.2 - 7.5; 8	
	Th	29	Cont: Steady State Non-Isothermal Reactor Design; Review	8	
Nov	T	3	Steady State Non-Isothermal Reactor Design	8	HW 6 Due
	Th	5	Exam 2		Exam 2
	T	10	Continue: Steady State Non-Isothermal Reactor Design	8	
	Th	12	Continue: Steady State Non-Isothermal Reactor Design	8	
	T	17	Continue: Steady State Non-Isothermal Reactor Design	8	
	Th	19	Catalysis and Catalytic Reactors	10	HW 7 Due
	T	24	Exam 3		Exam 3
	Th	26	No Class (Thanksgiving)		
Dec	T	1	Cont. Catalysis and Catalytic Reactors	10	
	Th	3	Cont. Catalysis and Catalytic Reactors	10	HW 8 Due
	T	8	Review		
	T	15	Final Exam (08:00-10:00)		Final Exam

Below is a **brief** list of issues that are frequently encountered, including examples from a CHEE 203 HW assignment. Please read the following information carefully before completing your next homework assignment. Significant point deductions may be applied to submitted assignments that are unprofessional. I strongly urge you to follow these recommendations for future classes or anything submitted for any kind of approval. Most of these items are common sense. Thank you to those of you that are already doing these things.

General standards for any submitted work

1. If you are turning in more than 1 sheet of paper – they should be **stapled**. They should **not be** loose or rolled up in a corner.

2. They should never have that frilly binder ring torn up edge.

3. Your name should be clearly written on the assignment (preferably in the top right). It is advisable to include assignment related information as well (Course Number, Assignment Number, Date). Subsequent pages should have your last name and page number on them as well.

4. All of your work should be legible and have some degree of organization to it. All answers should be clearly indicated with a box, double underline, or highlighted.

5. Problems should be separated from one another. If a problem only takes up a small portion of the page, leave a decent gap between the end of the problem and the start of the next one. If the problem takes up more than the majority of the page, start the next problem on a separate page.

6. Do not "continue" a problem after the start of another one. This goes along with the previous statement – leave yourself room to make adjustments or edits if needed.

7. Each problem should be separated into a nice flow of how you got from the data you're given, to the final answer you've come up with.

8. Use an eraser if you want to remove what you've written in pencil. Do not just scribble over what you've already written down. If you've written in pen and made a mistake, draw a line through your error, or if a large portion of the page is incorrect, start a new page.

Problem specific standards for any submitted work

9. If you need to solve an intermediate step (e.g. temperature dependent density to input into your final equation), the work for this should be included and the intermediate answer should be clearly indicated. If this value is looked up in a table or an appendix, you should at least indicate this. The source of any looked up value should be cited.

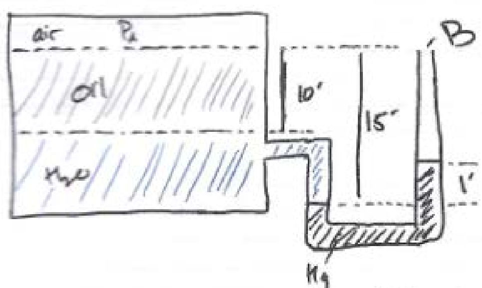
10. Sketches should be included where appropriate. Any variables you define should be included in the sketch – especially dimensions. If a sketch is given in the problem statement, it is fine to copy or print out the sketch and annotate it.

11. If you use a variable that is not given in the problem statement – it should be clearly defined as to what it is. Any assumptions need to be clearly stated.

12. Any time a variable is switched to its value, the units should be carried through with it to the final answer.

13. All work needs to be clearly shown, draw attention to important work and intermediate values with underlines, circles, or boxes.

These are examples of a clear and concise problems with appropriate sketches when necessary.



$SG_{oil} = 0.8$

$\rho_{oil} = 800\ kg/m^3$

$\rho_{H_2O} = 1000\ kg/m^3$

$\rho_{Hg} = 1360\ kg/m^3$

$1' = 0.3048 m$

$5' = 1.524 m$

$10' = 3.048 m$

Point B: $P_{atm} + g(1'\rho_{Hg})$

Point A: $P_A + g[10'\rho_{oil} + 5'\rho_{H_2O}]$

Point A = Point B

$$P_A + g[10'\rho_{oil} + 5'\rho_{H_2O}] = P_{atm} + g(1'\rho_{Hg})$$

$$P_A = P_{atm} + g(1'\rho_{Hg}) - g[10'\rho_{oil} + 5'\rho_{H_2O}]$$

$$= P_{atm} + g[1'\rho_{Hg} - 10'\rho_{oil} - 5'\rho_{H_2O}]$$

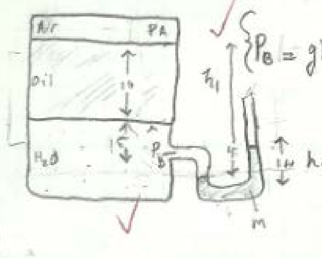
$$= 1 atm + 9.8\frac{m}{s^2}\left[0.3048 m\left(\frac{13600 kg}{m^3}\right) - 3.048 m\left(\frac{800 kg}{m^3}\right) - 1.524 m\left(\frac{1000 kg}{m^3}\right)\right]$$

$$= 1 atm + 9.8\frac{m}{s^2}\left(182.88\frac{kg}{m^2}\right) = 1 atm + 1792.22\ Pa\left(\frac{1 atm}{101325\ Pa}\right)$$

$$= 1 atm + 0.01768\ atm$$

$$\boxed{P_A = 1.018\ atm}$$

5)



$10 ft = 3.048 m$

$5 ft = 1.542 m$

$\rho_{H_2O} = 1000\ kg/m^3$

$\rho_{oil} = 800\ kg/m^3$

$$\left\{ P_B = g h_2 \rho_m + (1) = P_A + \rho_{oil}\, g\,(3.048\,m) + \rho_{H_2O}\, g\,(1.542\,m) \right\}$$

(1) in Atm

$$(9.8\tfrac{m}{s^2})(0.304\,m)(13600\tfrac{kg}{m^3}) + 1 = P_A + (800\tfrac{kg}{m^3})(9.8\tfrac{m}{s^2})(3.048\,m) + (1000\tfrac{kg}{m^3})(9.8\tfrac{m}{s^2})(1.5)$$

1 in atm; 1 atm =

$$39{,}984_{Pa} + 101{,}325_{Pa} = P_a + 39{,}007.92_{Pa}$$

$$\boxed{P_a = 102{,}302.08\ P_A = 1.01\ atm}$$

★ Pressure

$$\frac{dP}{dz} = \frac{-P \cdot MW}{RT}$$

$$\Rightarrow \frac{dP}{P} = \frac{-MW}{RT}\,dz$$

★ Temp as a function of Pressure ★

$$T_2 - T_1 = m\,(P_2 - P_1) \quad \leftarrow \text{slope}$$

$$\Rightarrow \boxed{m = \frac{T_2 - T_1}{P_2 - P_1} = \text{slope}}$$

$$T - T_A = m\,(P - P_A)$$

$$\Rightarrow \boxed{T = T_A + m\,(P - P_A)}$$

or can use $T = f(z)$

$$MW_{dry\ air} = 28.97 \times 10^{-3}\ kg\ mol^{-1}$$

$$-\frac{MW}{R}\,dz = \frac{T}{P}\,dP$$

$$\Rightarrow -\frac{MW}{R}\,dz = \frac{T_A + m(P - P_A)}{P}\,dP$$

For this problem, our R constant will be $8.206 \times 10^{-5}\ m^3\,atm\,K^{-1}\,mol^{-1}$

$$-\frac{MW}{R}\int_{z_A}^{z_B} dz = \int_{P_A}^{P_B} \frac{T_A + m(P - P_A)}{P}\,dP$$

$$-\frac{MW}{R}(z_B - z_A) = \int_{P_A}^{P_B} \frac{T_A}{P}\,dP + m\left[\int_{P_A}^{P_B} \frac{P}{P}\,dP + \int_{P_A}^{P_B} \frac{-P_A}{P}\,dP\right]$$

($z_A = 0$)

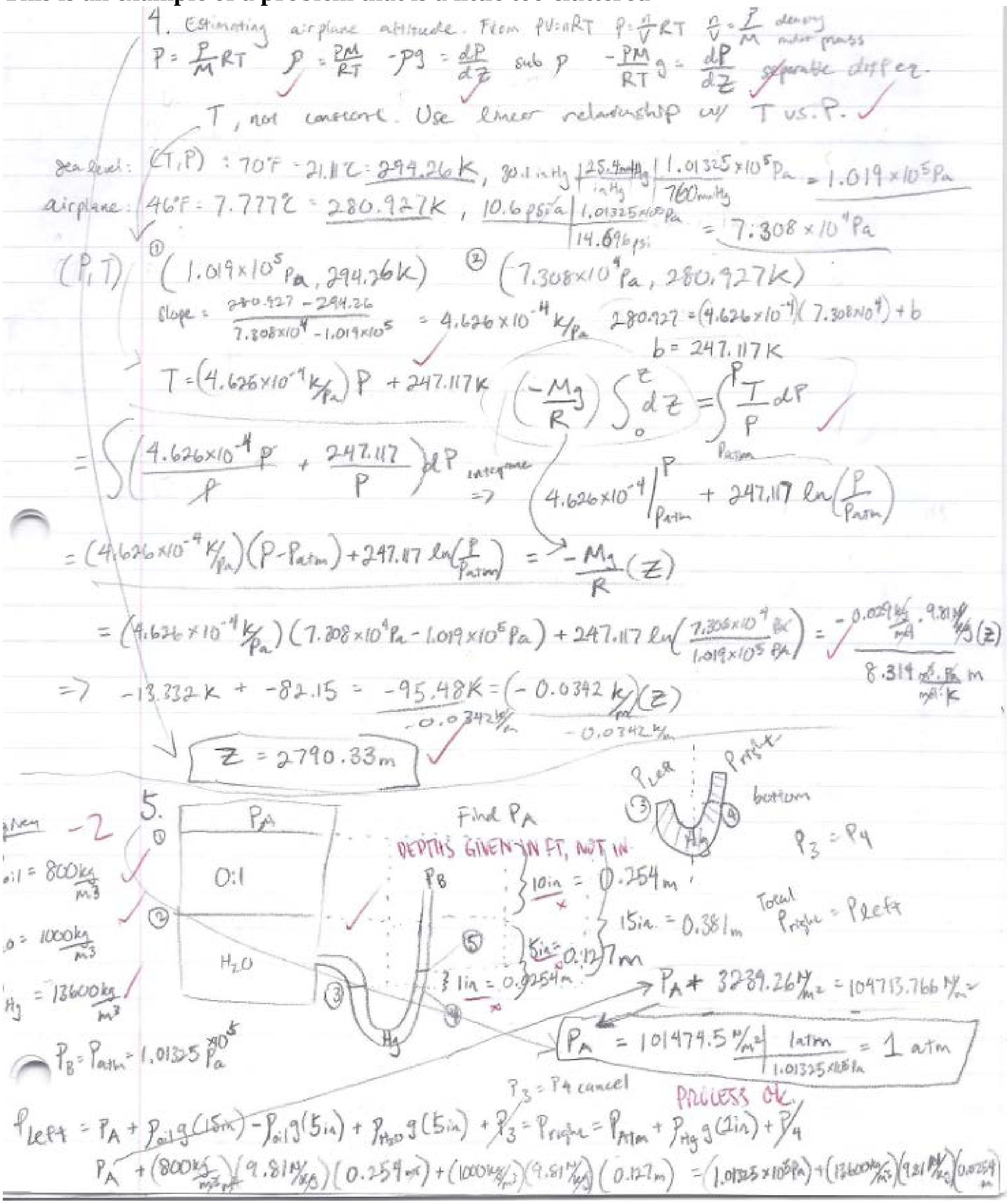
$$-\frac{MW z_B}{R} = T_A \ln\left|\frac{P_B}{P_A}\right| + m\left[(P_B - P_A) - P_A \ln\left|\frac{P_B}{P_A}\right|\right]$$

$$\Rightarrow z_B = \frac{-R}{MW}\left[T_A \ln|P_B/P_A| + m\cdot[(P_B - P_A) - P_A \ln|P_B/P_A|]\right]$$

where $P_B = 73064\ Pa$, $P_A = 101{,}918.6\ Pa$, $T_A = 294.261\ K$ | $MW = 28.91\ kg\ mol^{-1}$

$$\Rightarrow \boxed{z_B = \sim 2800\ m \quad \text{or} \quad 2.8\ km}$$

This is an example of a problem that is a little too cluttered



4. Estimating airplane altitude. From $PV=nRT$ $P=\frac{n}{V}RT$ $\frac{n}{V}=\frac{\rho}{M}$ density / molar mass

$P=\frac{\rho}{M}RT$ $\rho=\frac{PM}{RT}$ $-\rho g=\frac{dP}{dz}$ sub ρ $-\frac{PM}{RT}g=\frac{dP}{dz}$ separable diff eq.

T, not constant. Use linear relationship w/ T vs. P.

sea level: (T,P) : 70°F = 21.1°C = 294.26 K, 30.1 inHg $\left|\frac{25.4\,mmHg}{in\,Hg}\right|\frac{1.01325\times10^5 Pa}{760\,mmHg} = 1.019\times10^5 Pa$

airplane: 46°F = 7.777°C = 280.927 K, 10.6 psia $\left|\frac{1.01325\times10^5 Pa}{14.696\,psi}\right| = 7.308\times10^4 Pa$

(P,T) ① $(1.019\times10^5 Pa, 294.26K)$ ② $(7.308\times10^4 Pa, 280.927K)$

Slope = $\frac{280.927-294.26}{7.308\times10^4-1.019\times10^5} = 4.626\times10^{-4} K/Pa$ $280.927=(4.626\times10^{-4})(7.308\times10^4)+b$

$b = 247.117K$

$T=(4.626\times10^{-4} K/Pa)P + 247.117K$ $\left(-\frac{Mg}{R}\right)\int_0^z dz = \int_{P_{atm}}^{P}\frac{T}{P}dP$

$= \int\left(\frac{4.626\times10^{-4}P}{P} + \frac{247.117}{P}\right)dP$ integrate ⇒ $4.626\times10^{-4}\Big|_{P_{atm}}^{P} + 247.117\ln\left(\frac{P}{P_{atm}}\right)$

$=(4.626\times10^{-4} K/Pa)(P-P_{atm}) + 247.117\ln\left(\frac{P}{P_{atm}}\right) = -\frac{Mg}{R}(z)$

$=(4.626\times10^{-4} K/Pa)(7.308\times10^4 Pa - 1.019\times10^5 Pa) + 247.117\ln\left(\frac{7.308\times10^4 Pa}{1.019\times10^5 Pa}\right) = -\frac{0.029\,kg/mol \cdot 9.81\,m/s^2}{8.314\,\frac{m^3\,Pa}{mol\,K}}(z)$

⇒ $-13.332K + -82.15 = -95.48K = (-0.0342\,K/m)(z)$

$z = 2790.33m$

5. Find P_A

DEPTHS GIVEN IN FT, NOT IN

P_A / oil / H_2O / Hg; ① ② ③ ④ ⑤; P_B

10 in = 0.254 m; 15 in = 0.381 m; 5 in = 0.127 m; 1 in = 0.0254 m

P_{left}, P_{right}, bottom ③ ④, Hg; $P_3 = P_4$; Total $P_{right} = P_{left}$

-2

oil = 800 kg/m³; H_2O = 1000 kg/m³; Hg = 13600 kg/m³

$P_B = P_{atm} = 1.01325\times10^5 Pa$

$P_A + 3239.26\,N/m^2 = 104713.766\,N/m^2$

$P_A = 101474.5\,N/m^2 \left|\frac{1atm}{1.01325\times10^5 Pa}\right. = 1\,atm$

PROCESS OK.

$P_3 = P_4$ cancel

$P_{left} = P_A + \rho_{oil}g(15in) - \rho_{oil}g(5in) + \rho_{H_2O}g(5in) + P_3 = P_{right} = P_{atm} + \rho_{Hg}g(1in) + P_4$

$P_A + (800\,kg/m^3)(9.81\,N/kg)(0.254\,m) + (1000\,kg/m^3)(9.81\,N/kg)(0.127m) = (1.01325\times10^5 Pa) + (13600\,kg/m^3)(9.81\,N/kg)(0.0254\,m)$