### Purdue University CHE 20500: Chemical Engineering Calculations, Fall 2023

- **A.** Instructor. Professor Liu (julieliu@purdue.edu) and Professor Morgan (jamorgan@purdue.edu)
- **B.** Catalog Description. Quantitative applications of steady-state mass and energy balances to solve problems involving multi-component systems and multi-unit chemical processes. Single-component and multi-component phase equilibria, single-reaction and multiple-reaction stoichiometry, coupled mass and energy balances, chemical processes involving bypass and recycle streams.
- C. Prerequisites. Chemistry 116 or Chemistry 136; Mathematics 161 (or equivalent); Physics 172 (or equivalent)
- **D.** Course Text. Elementary Principles of Chemical Processes, 4<sup>th</sup> Edition with the WileyPlus account by R. M. Felder, R. W. Rousseau, and L. G. Bullard. Wiley and Sons, 2016. Purchases can be made through the bookstore or directly from Wiley.
  - WileyPLUS Access with downloadable eText ISBN: 9781119498704
  - WileyPLUS Access with downloadable eText and Loose Leaf 1 semester ISBN: 9781119760818
- **E.** Course Learning Objectives. It is expected that, by the conclusion of the semester, class participants should be able to:
  - Work professionally and ethically as a member of a chemical engineering team.
  - State and describe the diverse social, economic, and environmental issues associated with being a chemical engineer.
  - Apply the law of conservation of mass and conservation of atomic species in order to solve mass balances in unit operations with and without chemical reactions and with and without recycle streams.
  - Determine, using first principles and well-established correlations, the relations between thermodynamic equilibria and multiphase systems.
  - Integrate the first law of thermodynamics with the concept of energy balances in unit operations with and without chemical reactions and with and without recycle streams.
  - Apply the laws of conservation of mass and energy and thermodynamic equilibrium data in order to formulate solutions for mass and energy flow rates in multi-unit systems.
  - Utilize the concepts of transient mass balance problems in order to develop a basis for non-steady state applications.
  - Design multi-unit chemical processes using steady-state and transient mass and energy balances in order to create multi-unit operations similar to those in future courses and applications in industry.
- **F. Course Outcomes.** By the end of the course, the student should be able to:
  - 1. Estimate physical properties of real chemical systems (Utilized in CHE 21100, 30600, 34800, 37700, 37800, 42000, 43500, 45000)
  - 2. Evaluate introductory single-component and multi-component phase equilibria and incorporate these concepts into solutions of mass and energy balance problems (Utilized in CHE 21100, 30600, 37800, 43500, 45000)
  - 3. Solve steady state and transient mass and energy balance problems for both reacting and non-reacting systems with or without recycle using analytical and computational methods (Utilized in CHE 21100, 30600, 34800, 37700, 37800, 42000, 43500, 45000, 45600)
  - 4. Work professionally and ethically in teams to solve mass and energy balance problems (Utilized in CHE 30600, 34800, 37700, 37800, 43500, 45000)
  - 5. Identify contemporary chemical engineering problems, including their impact on societal, economic, public welfare, environmental, and global factors (Utilized in CHE 30000, 40000, 42000, 45000)

- **G.** Davidson School of Chemical Engineering Program Outcomes for ABET. Graduates of the Charles D. Davidson School of Chemical Engineering at Purdue University will (bolded items are addressed in this course):
  - 1. Apply principles of engineering, science, and mathematics to solve complex chemical engineering problems.
  - 2. Apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors.
  - 3. Communicate effectively with a range of audiences.
  - 4. Recognize ethical and professional responsibilities in chemical engineering situations and make informed judgments, which must consider the impact of engineering solutions in global, economic, environmental, and societal contexts.
  - 5. Function effectively on a team whose members together provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives.
  - 6. Develop and conduct appropriate experimentation, analyze and interpret data, and use engineering judgment to draw conclusions.
  - 7. Acquire and apply new knowledge as needed, using appropriate learning strategies.
- **H.** Expectations. This is a 4 credit hour course, and it is expected that each student will spend a minimum of 12 hours each week (3 hours per credit) outside of lectures working on homework, studying, reading the course text, and completing assessment questions. In many cases, the first year in the university is harder than high school, but it is manageable with noticeably less effort than described above. This class, and all subsequent chemical engineering classes, will be much more challenging, and hence more rewarding, than anything that most students will have seen in previous courses. We encourage you to take studying seriously and establish good study habits (e.g., read the text during the assigned week, practice using additional problems). This will lead to a successful start of the student's chemical engineering career.
- I. Instructors' Commitment. Your instructors will: (1) be courteous, punctual, well-organized, and prepared for class activities; (2) answer questions clearly in class or through office hours; (3) be available during office hours or notify you beforehand if they are unable to keep to the original office hour schedule; and (4) grade uniformly and consistently to the posted guidelines.
- **J. Consulting with the Faculty Members.** We encourage you to discuss academic or personal questions with us during office hours or via email. These discussions need not be limited to CHE 20500 content.
- K. Academic Dishonesty. Academic dishonesty will not be tolerated in any form in this course. Specifically, Purdue prohibits "dishonesty in connection with any University activity. Cheating, plagiarism, or knowingly furnishing false information to the University are examples of dishonesty." [Section B-2-a, Code of Student Conduct] Furthermore, the University Senate has stipulated that "the commitment of acts of cheating, lying, and deceit in any of their diverse forms (such as the use of substitutes for taking examinations, the use of illegal cribs, plagiarism, and copying during examinations) is dishonest and must not be tolerated. Moreover, knowingly to aid and abet, directly or indirectly, other parties in committing dishonest acts is in itself dishonest." [University Senate Document 72-18, December 15, 1972] All incidents of academic dishonesty will be reported to the Dean of Students. Such incidents include: (i) possessing or accessing, in hardcopy or electronic form, solutions to the: course text, previous years' homework problems, and exams (e.g., obtaining solutions from websites such as Course Hero, Chegg, Quizlet, etc.); (ii) claiming credit for work that is not your own original work; (iii) enabling other students to create work that is not their original work; and (iv) collaborating with other students (or getting other outside help) during an exam. The punishment for the first offense is a grade of zero for the entire work (exam, quiz, or homework), and the punishment for a second offense is an F mark for the class.
- L. Academic Integrity. Academic integrity is one of the highest values that Purdue University holds. Individuals are encouraged to alert your instructors and university officials to potential breeches of this value by either emailing integrity@purdue.edu or by calling (765) 494-8778. While information may be submitted anonymously, the more information that is submitted provides the greatest opportunity for the university to investigate the concern.

- M. Student-Initiated Purdue Honors Pledge. As a Boilermaker pursuing academic excellence, I pledge to be honest and true in all that I do. Accountable together we are Purdue.
- N. Student Professionalism. The highest standards of professionalism and ethics are expected in CHE 20500. Each student is expected to come to class on time and not disrupt the class. Each student is expected to follow Purdue's student conduct code and behave in a professional manner. The rights of students in violation of the code of conduct are outlined on Purdue's website. Each student is expected to exhibit consideration and respect towards the other students, the teaching assistants (TAs), the graders, and the faculty members. Each student is expected to exhibit a positive attitude. Expectations for each student include (but are not limited to):
  - a. Attending all class sessions.
  - b. Coming to class on time and prepared by reading assigned material beforehand.
  - c. Refraining from disrupting class (e.g., turning off or silencing mobile phones, refraining from mobile phone or laptop use during class, and carrying on a loud conversation during class).
  - d. Maintaining the highest standards of academic honesty and integrity.
  - e. Being an active contributor to team assignments.
  - f. Being knowledgeable about the policies and information described in the syllabus.
- O. Key Course Dates.

Lectures (face-to-face):	Wednesday and Friday	10:30 a.m. – 12:30 p.m.	WALC 3087
Exam 1	Thursday, September 21, 2023	8:00 p.m. – 9:30 p.m.	UC 114
Exam 2	Monday, October 23, 2023	8:00  p.m. - 9:30  p.m.	UC 114
Exam 3	Monday, November 20, 2023	8:00  p.m. - 9:30  p.m.	UC 114

Final Exam To Be Announced, As Set by the University

No Class 9/4 Labor Day

9/13, 11/8, 12/8 Make-up for Hour Exams 11/22, 11/24 Thanksgiving Break

Class Drop Deadline with a Withdrawal (W): Monday, November 27

- P. Emergency Procedure for the Wilmeth Active Learning Center (WALC). In the event that the class would need to evacuate WALC (e.g., in the event of a fire alarm), the class should proceed to exit the building and meet on the southeast corner of Potter Engineering Center (POTR). In inclement weather, meet in the lounge inside of the southeast corner of POTR. Do not leave the area as emergency responders will need to count to ensure that all persons have made it from the facility. In the event that we are required to shelter in place (e.g., due to a tornado warning), we will proceed to the appropriate shelter in place area within the basement level of WALC.
- Q. Office Hours
  - a. Professor Liu (julieliu@purdue.edu, Office: FRNY 1160)
    Office Hours (Location: FRNY 3062A): Tuesday, 11:00 am 12:00 pm
  - **b. Professor Morgan** (jamorgan@purdue.edu, Office: FRNY 1053) Office Hours (Location: FRNY 2142): Monday, 11:30 am 12:30 pm
  - c. Zachary Beickman (zbeickma@purdue.edu)
    Office Hours (Location: FRNY 1043): Monday, 6:30 pm 8:30 pm
  - **d.** Bryan Cruz Delgado (<u>bcruzdel@purdue.edu</u>) Office Hours (Location: PHYS 223): Tuesday, 5:00 pm – 7:00 pm
  - e. Marisa Egan (egan18@purdue.edu)
    Office Hours (Location: HAMP 3153): Wednesday, 5:00 pm 7:00 pm

- **R. Website for Course Information (purdue.brightspace.com/).** This course will use the Brightspace site. The website is limited to enrolled students and will have the syllabus, homework assignments, and other important class information associated with it. To login, use your university name and password. Please check the website regularly for assignments. Important announcements will be posted on the Brightspace page and will not be automatically sent to e-mail. To get an e-mail/text notification of new announcements, follow the directions <a href="here">here</a>.
- **S. E-mail.** Occasionally, important class announcements will be disseminated through the class e-mail list. It is your responsibility to regularly check your e-mail every day and to read the e-mails regarding CHE 20500 to receive important class information. E-mail is the preferred mode of contact. Please put CHE 205 in your subject line. If you e-mail the instructors with questions or a request to make an appointment, please allow a minimum of 24 hours for a response during the week or a response by Monday at 5 pm if the e-mail is sent on the weekend.
  - Assessment of Course Outcomes. A weighted average grade will be calculated as follows.

Concept Quizzes: 2% Examinations: 20% each = 60% total

Homework: 13% Final Examination: 25%

### The grading scale will be as follows.

T.

A range: 100 - 85% of the weighted points B range: 84.9 - 75% of the weighted points C range: 74.9 - 65% of the weighted points D range: 64.9 - 55% of the weighted points F: Less than 55% of the weighted points

If an exam or homework was too difficult (as judged by the faculty instructors), the final course grade may be scaled to a higher value. Grades will never be scaled downward. As a rule, scaling will not be applied. There is no preset distribution of final grades. The grading will reflect demonstrated student capability relative to an absolute performance standard that is expected of all Purdue chemical engineering students, rather than a scale that compares students to a mean performance metric on any evaluation vehicle. In practice, this means the entire class could receive A marks.

- **U. Concept Quizzes.** There will be concept quizzes assigned through Wiley Plus. The quizzes are open notes and open book but must be done on your own. You cannot work with others on the quizzes.
- V. Electronic Homework. Electronic homework will be performed in groups and turned in via Gradescope. <u>Begin each problem on a new sheet of paper, and number the pages</u>. The solution to each problem <u>must</u> include a picture or flow chart (hand or computer-generated) of the system or problem of interest, a listing of the known quantities and their units of measurement, and a listing of the unknown quantities that must be determined. <u>If your solution to a problem does not contain these items, it will not be graded and you will receive a grade of 0 for that problem.</u> The homework will be representative of content posed on the midterm and final examinations. As such, the purpose of the homework is to ensure that learners are comfortable with the course content. Homework solutions will not be posted. It is your responsibility to get help either before the problems are due or after they have been submitted for grading.
- W. Late Homework. All assignments are due on the stated date and time given when the homework is assigned. <u>Late homework will not be accepted.</u>
- X. Homework Grading. Homework will be graded on the basis of 10 points per problem. A problem worked perfectly or with 1 or 2 minor errors will get 10 points. A problem with more than 2 minor errors but no major (logic) errors will get 7.5 points. A problem with 1 major error or more than 3 minor errors will get 5 points. A problem with more than 1 major error will get 2.5 points. A problem with no credible effort will get zero points. The assessment of your performance and contribution by your teammates will be used to scale your homework grades. Your lowest scaled homework score will be dropped.

- Y. Team Evaluations. An ability to function effectively on teams is a learning objective of this course. Students will be assigned to two different teams during the semester to complete homework assignments. The first team pairing will be for the first half of the assignments, and the second team pairing will be for the second half of the assignments. Students will use CATME to submit information used for Team Formation and Peer and Team Evaluations. At the end points of each team pairing, students will be required to log into CATME and rate their performance as well as the performances of their team members. Each student's point total for the team homework assignments completed in that timeframe will be multiplied by the multiplier to obtain the final point total for those homework assignments. The CATME software will use the evaluations to compute a "multiplier" with a value between 0.00 (very poor contributions to group) and 1.05 (extremely excellent contributions to group) for each group member. If one is interested in how these multipliers are calculated, please see the research papers posted at https://info.catme.org/research/. Note that multipliers of 0.00 are very rare; typically, multipliers are between 0.80 and 1.05.
- **Z. Homework Cover Page.** Each homework assignment must have a cover sheet. A template of the cover sheet is posted on Brightspace (in the Homework module) as a fillable Microsoft Excel sheet. The cover sheet <u>must contain</u> the printed first and last names of the group members, the date, and the homework assignment number in the appropriate locations. Below this identifying information, the following statement MUST appear:

"Each signature below attests that the signer contributed significantly to the solution of all problems in this homework assignment".

All team members who contributed must sign and print their names next to the signature. The signature and printed names must be clearly legible. IF A TEAMMATE DID NOT PARTICIPATE IN THE SOLUTION OF THE HOMEWORK, THEN THIS TEAMMATE SHOULD NOT SIGN. If multiple groups worked together, indicate that on the cover page. Otherwise, identical solutions will be regarded as cheating. If this page is not present, the homework will be awarded a grade of zero and will be returned ungraded. If a team member does not participate in the solution of all the problems on the assignment, that team member will receive a grade of zero on the entire homework assignment.

AA. Examinations. Timed examinations will be conducted in person. For each examination you will be supplied with one or more pages of relevant equations. You will not be allowed to use any books or notes in addition to these equations pages, which means that all you will be allowed to have on your desk during the examination period is: the exam itself, the notes pages provided, the paper on which you are writing solutions, something with which to write, and a calculator. All other electronic devices are forbidden, including cell phones and pagers. These must be turned off and may not be handled at any time during the exam. Students caught with other materials during an exam will be assumed to be cheating. Remember that no collaboration or outside help is allowed. The final exam is comprehensive (i.e., it will cover the entire contents of the course).

Any student who cannot take an exam as scheduled (e.g., religious holiday, conflicts with another exam) *must* make special arrangements by sending the instructors an e-mail at least one month *before* the exam is given. In cases of extenuating circumstances (e.g., illness, quarantine, bereavement) or extreme duress (e.g., hospitalization), please provide documentation to Prof. Liu or Prof. Morgan, and if possible, speak to one of the instructors *before* the exam takes place. Travel plans do not constitute extenuating circumstances.

- **BB.** Regrade Requests for Homework and Exams. A student <u>has one week after the graded exam or homework has been released</u> to submit a regrade request via Gradescope. This is the only means by which to have work re-graded in this course. Any homework assignments or exams submitted for re-grading will be *re-graded in their entirety* and may be marked lower than the original score that was received. For exams, regrade requests will not be accepted until after the exam solutions have been posted and students have compared their solutions to the posted solutions.
- CC. Accessibility. Purdue University strives to make learning experiences accessible to all participants. If you anticipate or experience physical or academic barriers based on disability, you are welcome to let us know so that we can discuss options. You are also encouraged to contact the Disability Resource Center at: drc@purdue.edu or by phone: (765) 494-1247. If you are a student with any form of individual learning needs, please speak with the professors whether or not you seek an accommodation so that we are aware of your circumstance and can deliver course content in a manner that is most compatible with your learning situation.

In addition to the University policy, the Davidson School of Chemical Engineering has established procedures for students seeking accommodations. These can be found online at the ChE Undergrad Office website. Only those accommodation requests that conform to both University and ChE policy guidelines will be implemented.

Some important points from the ChE policy include: Please give letters of accommodation to Prof. Liu, Prof. Morgan, and your academic advisor (and not the graduate TA for office hours). If you have your letter at the start of the term, we strongly recommend you give it to us within the first two weeks of the semester. If your accommodation involves exam conditions, we strongly urge you to provide a minimum of one week notice to ensure that the accommodations requested are available.

**DD.** Campus Emergencies. In the event of a major campus emergency, course requirements, deadlines, and grading percentages are subject to changes that may be necessitated by a revised semester calendar or other circumstances beyond the instructor's control. Here are ways to obtain information about changes in this course. You are expected to check your @purdue.edu email address frequently.

Course Brightspace Page: Fall 2023 CHE 20500-003 LEC

Instructors' email addresses: julieliu@purdue.edu, jamorgan@purdue.edu

- **EE.** Nondiscrimination Statement. Purdue University is committed to maintaining a community that recognizes and values the inherent worth and dignity of every person; fosters tolerance, sensitivity, understanding, and mutual respect among its members; and encourages each individual to strive to reach his or her own potential. In pursuit of its goal of academic excellence, the University seeks to develop and nurture diversity. The University believes that diversity among its many members strengthens the institution, stimulates creativity, promotes the exchange of ideas, and enriches campus life. A hyperlink to Purdue's full Nondiscrimination Policy Statement is included in our course Brightspace under University Policies and Statements.
- FF. Attendance. This course follows the Academic Regulations: Attendance and Office of the Dean of Students: Class Absences policy posted in Brightspace under "University Policies and Statements." This policy states that students are expected to be present for every meeting of the classes in which they are enrolled. It is understood that, occasionally, you may miss lecture due to unforeseen circumstances (e.g., illness please do not come to class if you are feeling ill), and, in these cases, you can ask any questions about missed concepts during office hours. Unless it falls under the University excused absence regulations (see below), any work due should be submitted on time. In cases falling under excused absence regulations, the student or the student's representative should contact or go to the Office of the Dean of Students (ODOS) website to complete appropriate forms for instructor notification. Under academic regulations, excused absences may be granted by ODOS for cases of grief/bereavement, military service, jury duty, parenting leave, or emergent medical care.
- **GG. Illness.** If a student becomes sick (e.g., with flu-like symptoms), the student should seek prompt medical attention, and then not come back to class until the student has been symptom-free for more than 24 hours. That is, the student should utilize the resources at the Purdue University Student Health Center (PUSH) or another trained medical professional. Materials will be made available electronically to assist any students who are ill, and reasonable accommodations will be made on an individual basis to ensure that all students have the opportunity to learn. If possible, the student should let Professor Liu and Professor Morgan know as soon as possible such that they can aid in bringing the student up to speed in the course material as rapidly as possible. In the event of a severe outbreak of illness at Purdue that mandates class not meet, all attempts will be made to deliver the course online.
- HH. Mental Health/Wellnes Statement. Purdue University is committed to advancing the mental health and well-being of its students. If you or someone you know is feeling overwhelmed, depressed, and/or in need of support, services are available. For help, such individuals should contact <u>Counseling and Psychological Services (CAPS)</u> at (765) 494-6995 during and after hours, on weekends and holidays, or through its counselors physically located in the Purdue University Student Health Center (PUSH) during business hours.
- II. Basic Needs Security. Any student who faces challenges securing their food or housing and believes this may affect their performance in the course is urged to contact the Dean of Students for support. There is no appointment needed and Student Support Services is available to serve students 8 am 5 pm Monday through Friday.

- JJ. Use of Copyrighted Materials. Among the materials that may be protected by copyright law are the lectures, notes, and other material presented in class or as part of the course. Always assume the materials presented by an instructor are protected by copyright unless the instructor has stated otherwise. Thus, these materials cannot be posted online (e.g., Chegg, Course Hero, etc.). Students enrolled in, and authorized visitors to, Purdue University courses are permitted to take notes, which they may use for individual/group study or for other non-commercial purposes reasonably arising from enrollment in the course or the University generally. Notes taken in class are, however, generally considered to be "derivative works" of the instructor's presentations and materials, and they are thus subject to the instructor's copyright in such presentations and materials. No individual is permitted to sell or otherwise barter notes, either to other students or to any commercial concern, for a course without the express written permission of the course instructor. To obtain permission to sell or barter notes, the individual wishing to sell or barter the notes must be registered in the course or must be an approved visitor to the class. Course instructors may choose to grant or not grant such permission at their own discretion, and may require a review of the notes prior to their being sold or bartered. If they do grant such permission, they may revoke it at any time, if they so choose.
- **KK. Disclaimer.** This syllabus is subject to change. If any change occurs, it will be announced in the class and/or posted on Brightspace.

### LL.Course Material as Listed by Topic.

- 1. Materials Balances
  - a. Open and Closed Systems
  - b. Steady-state Systems
  - c. Systems in a Transient State
  - d. Multi-unit Systems
  - e. Balances on Reactive Systems
  - f. Balances on Multiphase Systems
- 2. Solution Thermodynamics
  - a. Raoult's and Henry's Laws
  - b. Binary Vapor-Liquid Equilibrium

- 2. Solution Thermodynamics (Continued)
  - c. Binary Liquid-Liquid Equilibrium
  - d. Vapor-Liquid-Liquid Equilibrium
- 3. Energy Balances
  - a. First Law of Thermodynamics
  - b. Balances on Non-reactive Processes
  - c. Balances on Reactive Processes
- 4. Combined Mass and Energy Balances in Systems in a Transient State

### MM. Course Material as Listed by Text Chapter.

Chapters 1, 2, and 3 (self-taught)

Chapter 4: Fundamentals of Material Balances

Chapter 5: Single Phase Systems

Chapter 6: Multiphase Systems

Chapter 7: Energy and Energy Balances

Chapter 8: Balances on Nonreactive Processes

Chapter 9: Balances on Reactive Processes

Chapter 10: Balances on Transient Processes

### ChE 30600 Design of Staged Separation Processes Fall 2023

#### A. Instructor:

Professor Enrico Martinez FRNY G015 (765) 496-6998 marti309@purdue.edu Office Hours: Tuesdays 4:30-6:00, other times by appointment

### **B.** Teaching assistants:

Yen-Chun Lu Zhichen Nian Gabriel Perez Schuster

Office Hours: Mondays 2:20- 3:50, Room Forney 2142

C. Importance. Separation processes constitute 50% to 90% of the cost (capital and operating) of most chemical plants with distillation being the most commonly used separation method in the chemical and petroleum industries. Separations/mass transfer operations are one of the key items that distinguish chemical engineering from other engineering disciplines.

Classes will meet on Mondays and Wednesdays and some Fridays.

- **D. Goals.** The goal of this course is to apply the principles of mass conservation, energy conservation, phase equilibrium and mass transfer to achieve separations. The concepts and techniques will subsequently be used in ChE 43500 (Chemical Engineering Laboratory) and ChE 45000 (Design and Analysis of Processing Systems). Understanding of separation processes requires a thorough knowledge of mass balances, energy balances, thermodynamics and mass transfer you must have completed ChE 20500 (C or better) and ChE 21100.
- **E. Course Objectives.** Apply mass balances, energy balances, mass transfer and phase equilibrium to design and analyze separation processes.

### F. Course Outcomes.

- Utilize the concepts and relations of phase equilibria, particularly Vapor Liquid Equilibrium, in the analysis, design, and simulation of separation processes (21100→); (→43500, 45000)
- Use mass and energy balances in the analysis of separation processes
- Use the McCabe-Thiele diagram for the solution of problems in binary separations  $(\rightarrow 43500, 45000)$

- Use reflux and multi-stage cascades to increase separation of a given component  $(20500 \rightarrow)$ ;  $(\rightarrow 43500, 45000)$
- Use process simulators for binary and multi-component systems to solve, understand, and design separation processes (→43500, 45000)
- Apply the basic principles of distillation, absorption/stripping, and other unit operations for the solution of problems in separations (21100→); (→37800, 43500, 45000)
- Identify the safety aspects of various separation processes ( $\rightarrow$ 42000, 43500, 45000)
- Communicate effectively the results of a designed separation process in writing.
   (→43500, 45000)

### **G.** Anticipated Course Content

1. Introductory Material 1 week
2. Flash Distillation
3. Binary Distillation
4. Multi-Component Distillation
5. Complex Distillation Methods 1-2 weeks
6. Batch Distillation
7. Staged and Packed Column Design 1 week
6. Absorption/Stripping 1-2 weeks
7. Mass Transfer Analysis NTU-HTU Method. 1 week
8. Extraction
9. Membrane Separations
10. Adsorption Separations

## **H. Text:** P. C. Wankat, *Separation Process Engineering*, 5th edition, Prentice Hall, 2022. Print or e-Book:

9780137468041: Wankat: Separation Process Engineering 5e (Print) 9780137921324: Wankat: Separation Process Engineering 5e (Pearson+)

#### I. Software:

During this class, students will gain a working knowledge of the *Aspen Plus* process simulation package.

J. Grading Policy:	
Three One Hour Examinations (150 points each)	. 450 points
Individual Homework Assignments	. 150 points
Lab Performance/Reports	150 points
Team Design Project	150 points
TOTAL	900 points

Course grades will be determined from the adjusted course scores on the following basis:

Adjusted Course Score	Course Grade
90 and higher	A- [at least]
80 - 89	B- [at least]
70 - 79	
$60 - 69 \dots$	D- [at least]
Less than 60	F

Course Final grades for this class will be assigned using the +/- system (A+, A, A-, B+, B, etc...)

### K. Homework:

Assignments will be posted to Brightspace most Wednesdays after lecture time and are due in completed form by the following Wednesday, beginning of lecture. Late homework will be assessed a penalty of 5 pts if turned in by 6:30 PM. If not received by 6:30, you will receive no credit for that assignment. All late homework should be turned in to one of the teaching assistants. While you may find it helpful to discuss problem sets with one another, what you turn in must be your own work. Written homework's are to be done on Engineering Paper. For team assignments, write the team number and members name on the left top of each page, the course number (CHE 306) at the top middle of each page and the date on the right top of each page. Your homework's are to be neat and legible. Write on one side of the paper only.

### L. Exams

There will be three midterm exams during the semester (September 14, October 17 and November 14, 50 minutes long all evening exams, the first two in PHYS 112 and the third split into RAWL 1086, KRAN G016 AND KRAN 250.

Occasionally students will have to miss an intra-semester exam for personal or uncontrollable reasons. However, if an exam needs to me missed, there will NOT be a makeup exam given during the regular semester. Instead, the final exam will act as a make-up exam. PLEASE NOTE: A student can only miss a midterm exam for a legitimate reason (death in the family, illness, emergency, etc.) and ONLY if given permission by Professor Martinez. If a student attends all three exams during the semester, the final exam will not have to be taken.

#### M. On-line Course Evaluation

It is important for department and instructors to receive thorough feedback on all courses taught, so it is your responsibility to provide such feedback. Participation in the on-line course evaluation is mandatory and will be treated as a homework assignment worth 50 points.

### N. Design Project:

There will be one design project in the second half of the semester. The project will be done in teams of 3 students each. Further details of the project will be supplied after the third midterm exam.

### O. Student Expectations.

This is a 3-credit hour course, and it is expected that each student will spend 9 hours each week working on homework, studying, and reading the course text (3 hours/credit). This class, and all subsequent chemical engineering classes, will be much more challenging than you are likely used to, and at the same time much more rewarding than anything that most students will have seen before. We encourage you to take studying seriously and establish good study habits such as previewing the reading material *before* the lectures and practicing additional problems.

### P. Instructors' Commitment.

Your instructor will: 1) be courteous, punctual, well-organized, and prepared for lecture and other class activities; 2) answer questions clearly in class or arrange for detailed discussions out of class if in-class answers are not suitably clear; 3) be available during office hours or notify you beforehand if we are unable to keep them; 4) provide a suitable guest lecturer when we are traveling; and 5) grade uniformly and consistently to the posted guidelines.

### Q. Consulting with the Faculty Member.

We encourage you to discuss academic or personal questions with me during my office hours or via email or Hotseat. These discussions need not be limited to ChE 30600 content.

### R. Academic Dishonesty.

Academic dishonesty *will not be tolerated* in any form in this course. Specifically, Purdue prohibits "dishonesty in connection with any University activity. Cheating, plagiarism, or knowingly furnishing false information to the University are examples of dishonesty." [Section B-2-a, Code of Student Conduct] Furthermore, the University Senate has stipulated that "the commitment of acts of cheating, lying, and deceit in any of their diverse forms (such as the use of substitutes for taking examinations, the use of illegal cribs, plagiarism, and copying during examinations) is dishonest and must not be tolerated. Moreover, knowingly to aid and abet, directly or indirectly, other parties in committing dishonest acts is in itself dishonest." [University Senate Document 72-18, December 15,

1972] All incidents of academic dishonesty will be reported to the Dean of Students. Such incidents include: i) possessing or accessing, in hardcopy or electronic form, the solution manual to the course text, or to the exams, ii) claiming credit for work that is not your own original work, and iii) enabling other students to create work that is not their original work. The punishment for the first offense is a grade of zero for the entire work (exam or homework), and the punishment for a second offense is an F mark for the class.

#### S. Conduct.

University policy states that it is the responsibility of all students to attend all class sessions (http://www.purdue.edu/studentregulations/regulations\_procedures/classes.html). Each student is expected to come to class on time and not disrupt the class. Each student is also expected to follow Purdue's codes of student conduct

(http://www.purdue.edu/studentregulations/student\_conduct/regulations.html) and behave in a professional manner. The rights of students in violation of the code of conduct are outlined. Each student is expected to exhibit consideration and respect towards the other students, the graders, the teaching assistants (TAs), and the faculty member. Each student is expected to exhibit a positive attitude. Your conduct will be a factor in awarding grades to students between two letter grades. Purdue University's student conduct policy specifically addresses academic dishonesty.

### T. Violent Behavior Policy.

Purdue University is committed to providing a safe and secure campus environment for members of the University community. Purdue strives to create an educational environment for students and a work environment for employees that promote educational and career goals. Violent behavior impedes such goals. Therefore, violent behavior is prohibited in or on any University Facility or while participating in any University activity.

### U. Nondiscrimination.

Purdue University is committed to maintaining a community which recognizes and values the inherent worth and dignity of every person; fosters tolerance, sensitivity, understanding, and mutual respect among its members; and encourages each individual to strive to reach his or her own potential. In pursuit of its goal of academic excellence, the University seeks to develop and nurture diversity. The University believes that diversity among its many members strengthens the institution, stimulates creativity, promotes the exchange of ideas, and enriches campus life. Purdue University prohibits discrimination against any member of the University community on the basis of race, religion, color, sex, age, national origin or ancestry, genetic information, marital status, parental status, sexual orientation, gender identity and expression, disability, or status as a veteran. The University will conduct its programs, services and activities consistent with applicable federal, state and local laws, regulations and orders and in conformance with the procedures and limitations as set forth in Executive Memorandum No. D-1, which provides specific contractual rights and remedies. Any student who believes they have been discriminated against may visit www.purdue.edu/report-hate to submit a complaint to the Office of Institutional Equity. Information may be reported anonymously.

### W. Emergency Preparedness.

Purdue University is a very safe campus and there is a low probability that a serious incident will occur here at Purdue. However, it is important to emphasize the emergency procedures for evacuation and shelter-in-place incidents. Preparedness will be critical if an unexpected event is to occur. Emergency preparedness is your personal responsibility. Purdue University is actively preparing for natural

disasters or human-caused incidents with the ultimate goal of maintaining a safe and secure campus. The following is a review of the emergency procedures at Purdue University.

- 1. For any emergency call 911.
- 2. There are nearly 300 Emergency Telephone Systems throughout campus that connect directly to the Purdue Police Department (PUPD). If you feel threatened or need help, push the button and you will be connected to the PUPD.
- 3. If there is a fire alarm, we will immediately evacuate the building and proceed to in front of the WALC building. Do not use the elevator.
- 4. If there is a Shelter-in-Place requirement for a tornado warning, we will shelter in the lowest level of this building away from windows and doors.
- 5. If there is a Shelter-in-Place requirement for a hazardous materials release, we will shelter in the classroom shutting any open doors and windows.
- 6. If there is a Shelter-in-Place requirement for a civil disturbance, we will shelter in a room that is securable preferably without windows.

### X. Course Meeting Schedule.

Lectures: Monday, Wednesday, (some Fridays) 12:30 – 1:20, RHPH 172 Lab Sessions: Check Schedule according to your section

- **Y. Attendance.** University policy states that it is the responsibility of all students to attend all class sessions. You are expected to attend all lectures and recitation periods. (http://www.purdue.edu/studentregulations/regulations procedures/classes.html).
- **Z. Illness.** If a student becomes sick with flu-like symptoms, he/she should seek prompt medical attention, and then not come back to class until he/she has been symptom-free for more than 24 hours. A note from P.U.S.H., or another trained medical professional, is required to document illness. Materials will be made available electronically to assist any students who are ill, and reasonable accommodations will be made on an individual basis to ensure that all students have the opportunity to learn. In the event of a severe outbreak of illness at Purdue that mandates class not meet, all attempts will be made to deliver the course online through Blackboard.

**AA. Bereavement Policy.** Purdue recognizes that a time of bereavement is very difficult for a student. The University therefore provides rights to students facing the loss of a family member through the Grief Absence Policy for Students (GAPS): http://www.purdue.edu/odos/services/griefabsencepolicyforstudents.php. Students who find themselves in need of assistance in a time of bereavement should contact Professor Bao or Professor Martinez privately to discuss specific needs.

**BB.** Campus Emergencies. In the event of a major campus emergency, course requirements, deadlines and grading percentages are subject to changes that may be necessitated by a revised semester calendar or other circumstances beyond the instructors' control. Here are ways to get information about changes in this course. You are expected to check your @purdue.edu email address frequently.

### **CC. Individual Learning and Testing Needs.**

Any student who feels he/she may need an accommodation with any aspect of the course based on a personal circumstance should contact Professor Martinez privately to discuss his/her specific needs. If you are a student with any form of individual learning needs, please speak with the faculty instructor whether or not you seek an accommodation so that we are aware of your circumstance and can deliver course content in a manner that is most compatible with your situation.

# Purdue University ChE 348: Chemical Reaction Engineering (4 credit), Fall 2023 Syllabus

**Instructor:** Brian Tackett

Assistant Professor

**Chemical Engineering** 

Email: bmtacket@purdue.edu

**Office**: FRNY 2158 **Phone**: 765-496-7235

Office Hours: Mondays 4:30 – 6:00 pm, FRNY 2158

Teaching Assistants: Sarah Gustafson (gustaf14@purdue.edu),

Hwiyoon Noh (noh27@purdue.edu)

Office Hours: TBA

**Lecture Hours:** Mon/Wed/Fri

10:30 – 11:20 AM ARMS 1010

Synchronous, in-person

**Recitation Hours:** Recitation Section 1: Thu. 9:30 – 10:45 AM,

SC G064

Recitation Section 2: Thu. 11:30 AM – 12:45 PM,

CL50 129

<u>Laboratory Hours:</u> Lab Section 1 (9/14, 9/28, 10/12, 11/2): Thu. 9:30 – 11:20 AM,

FRNY G111

Lab Section 2 (9/14, 9/28, 10/12, 11/2): Thu. 11:30 AM – 1:20 PM,

FRNY G111

Website: Brightspace (CHE 348). All course materials will be posted on

Brightspace. It is your responsibility to keep up-to-date with all material posted online. All class announcements will be posted via Brightspace.

Required Text: H. S. Fogler, Elements of Chemical Reaction Engineering,

**SIXTH EDITION**, Prentice Hall, New York. ISBN 9780135486498.

Companion Website: http://websites.umich.edu/~elements/5e/

Course Description: Application of kinetic rate equations, mass balances and energy

balances to the analysis and design of chemical reactors involving homogeneous and heterogeneous chemical reactions. Chemical equilibria, kinetic rate equations for homogeneous and heterogeneously catalyzed reactions, design of ideal isothermal reactors, effects of non-isothermal operation, effects of diffusion in porous catalysts and non-

ideal mixing in continuous flow reactors.

**Prerequisites:** Chemical Engineering 211, Math Selective I, Chemistry 261

(concurrent)

**Learning Outcomes:** By the end of the course, students will be able to:

- 1. Apply fundamental material balances to derive the design equations for CSTR, PFR, PBR, and batch reactors.
- 2. Derive rate expressions from both elementary steps and reaction kinetics data for both homogeneous and heterogeneous reactions.
- 3. Use material and energy balances with kinetic data for both single and multiple reactions to design and analyze the behavior of isothermal and non-isothermal reactors.
- 4. Utilize effectiveness factors governing the coupling of reaction and diffusion in the description of heterogeneously catalyzed reactions.
- 5. Work professionally and ethically in teams to conduct reactionbased laboratory experiments.
- 6. Effectively report results in written form and practice safety as an integral part of laboratory work.
- 7. Apply appropriate computational tools for the solution of chemical reaction engineering problems.

### Technology Requirement:

Students are required to use computational software to solve reaction engineering problems for homework, project, and laboratory sessions. The TAs will provide training and support for **Python** and **Polymath** software. Other programs, such as MATLAB and Mathematica, may also be sufficient for solving the algebraic and ordinary differential equations encountered in this course, but the TA will not provide training for these methods. So it is recommended to use either Python or Polymath. Both programs are available on any FRNY computer lab machine (FRNY 1014, FRNY 1022, FRNY 1033, FRNY G023). You can also download software to use Python or Polymath on your personal computer:

- Python: is open source, free software. The most convenient way to get started with Python is to download Anaconda software from Anaconda.com. Follow download/install instructions on the website. Once installed, you can select the environment to run Python in. Spyder is a Python environment similar to MATLAB. Jupyter Notebooks is a Python environment in your web browser. Either will work.
- Polymath: is proprietary software developed specifically for the type of problems encountered in this course. You can access this software via AppsAnywhere by following instructions on this website:

https://engineering.purdue.edu/ECN/Support/KB/Docs/UsingAp psAnywhere.1.

### Recitations:

There are two recitation sections held each week. You may only attend the recitation section for which you are registered. Recitation will not be held during the weeks of laboratory experiments.

### **Laboratory:**

The Fundamentals Laboratory (FRNY G111) will be used to support this course. There are four weeks throughout the semester during which the lab periods, but not recitation, will be held. These lab period dates and the lab report due dates are listed in the calendar at the end of the syllabus. These dates are set, and it is not possible to schedule makeup labs. Please make every effort to attend your designated lab time.

<u>Lab reports are due two weeks following the lab experiment, by 11:59pm eastern time (on the day of your recitation).</u> One lab report per group must be uploaded to Gradescope.

The lab manual containing detailed information about the experiments and lab report guidelines can be found at the following link, and accessed using your Purdue career account login credentials: <a href="https://engineering.purdue.edu/Intranet/Groups/Schools/ChE/FundamentalsLabMaterials">https://engineering.purdue.edu/Intranet/Groups/Schools/ChE/FundamentalsLabMaterials</a>

If you need assistance gaining access to the Fundamentals Lab materials, more information can be found on Brightspace.

## <u>It is important that you read the lab manual one week in advance of your experiment.</u>

Part of the recitation sessions one week before the lab will also include a pre-lab activity, to discuss and prepare for the upcoming lab. For each lab report, each team member will be required to fill out a peer evaluation form and submit this via Gradescope, which will be used to adjust the lab grades assigned to each team member.

### A few reminders:

- Please read, sign, and bring the Fundamental Laboratory (FL) safety contract with you on the first day in the FL. You are required to complete the contract each time you start a new course in the FL.
- You are now required to bring your own safety glasses to the FL.
  The safety glasses should have side shields. You can use the
  goggles purchased for chemistry labs. If you need to purchase
  safety glasses, Follett's (across from Mackey Arena on
  Northwestern) stocks them.
- No coats, backpacks, or large bags are allowed into the FL.
   Students will not be permitted to leave their coats and backpacks
   outside the FL door, as was permitted in the past. You should
   have received an e-mail from Sandy Hendryx with your locker
   assignment for the year and locker combination. If you did not
   receive an e-mail with this information, please contact Sandy
   Hendryx (hendryxs@purdue.edu).

• The Fundamentals Lab is fully scheduled during the semester and therefore, we cannot conduct makeup lab sessions. If you miss a lab period for a valid reason, then your grade will be based on averaged grades from the other periods. Please show up 5 minutes early to your lab session. If you show up late to your lab period, you will be dismissed, and there will be no chance to make up missed labs. Missed lab periods without a valid reason will result in a zero grade. If you miss more than two lab periods without a valid reason, then you will be given an I or F grade for the course.

### **Course Grading:**

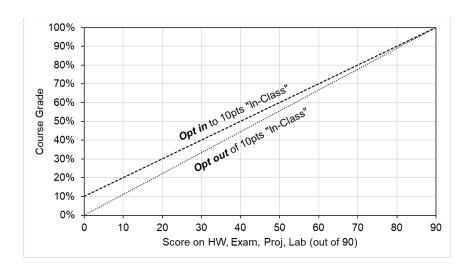
The final course grade will be determined by the following:

Lab Reports (4): 24 points
Exams (3): 27 points
Homeworks (14): 28 points
Final Project (1): 11 points
In-class: (10 points)

Individual assessments for each category are given equal weight (i.e. all 3 exams are weighted the same, all 14 homeworks are weighted the same, etc.). Individual assignments will be graded out of 100%, and the average percent for each category will determine the total class points for that category (e.g. an 80% average on exams yields 21.6/27 points).

10 Point In-class Option: This 10 points is for participating in "in-class" quizzes, clicker questions, and discussion. Credit is earned based on participation in these activities, and you can only earn the full 10 points by participating in >75% in-class activities. If you earn the 10 points, your grade will be calculated as the **opt in** scenario below. If you participate in <75% in-class activities, you will not be penalized, and your grade will be calculated as the **opt out** scenario below. You will automatically earn the 10 opt in points if you meet the >75% requirement (you do not have to request it). This grading scheme is meant to accommodate various learning styles.

Opt in: course grade = [(x + 10)/100] \* 100%
Opt out: course grade = [x/90] \* 100%
x = cumulative score on HW, Exams, Project, and Lab Reports



All grades will be available on Brightspace so that you can monitor your progress throughout the semester. Grades for individual homeworks, lab reports, and exams will **not** be adjusted by curving or scaling.

There is no preset distribution of final grades. The grading will reflect demonstrated student capability relative to an absolute performance standard that is expected of all Purdue ChE students, rather than a scale or curve that compares students to a mean performance metric on any evaluation vehicle. In practice, this means that if all students in the class demonstrate a high level of mastery of the course content, then all course grades could be A marks.

If your final numerical grade is greater than or equal to the following percentages, your letter grade is <u>guaranteed to be at least</u>:

A: ≥90%
B: ≥80%
C: ≥70%
D: ≥60%

Final numerical grades for the entire class may be scaled up (but never down). Plus and minus modifiers will be used to determine final grades.

### Exams:

**Exam 1:** Weds. Oct 4, 6:30pm – 7:30pm, KRAN G016 **Exam 2:** Mon. Nov 13, 6:30pm – 7:30pm, KRAN G016

Exam 3/Final: TBD

If students require approved accommodations for exams, these should be scheduled to be taken at the DRC in Stuart Hall. Students requiring accommodations are responsible for scheduling with the DRC prior to exam dates to ensure DRC availability.

### **Homework:**

Homework will be assigned via Brightspace, and will be **due on Gradescope at 11:59PM on Thursdays**. Late homework submissions

will be assigned a zero score. HW solutions will be posted to Brightspace when homeworks are graded (~1 week after due date).

Each HW problem will be graded on a scale of 2. 1 point will be earned for an honest attempt to solve the problem (beyond rewriting the problem statement). The remaining 1 point will be earned by correctly solving the problem, with partial credit given accordingly.

Scores on all HW assignments will be counted toward the course grade. **No HW grades will be dropped**.

**HW 0** counts for 2 full HW grades and consists of course evaluations: mid-term, and final evaluations. Each one must be completed by their respective dates in the course schedule in order to receive full credit for HW 0. These evaluations are critical to the success of the course and should be taken seriously.

Many homework problems will be assigned from the textbook. **Use of the textbook solutions manual is not permitted.** 

You may work on homework with other students in class, but you must submit your own individual assignment. You must also list the names of each person with whom you collaborated on a homework assignment.

### Regrade Requests:

You have <u>one week</u> after receiving a graded assignment to submit a regrade request. Requests must be made in-person to Prof. Tackett before or after lecture, or during office hours. Email requests may also be made to schedule an in-person meeting about regrading, as long as it is within one week of receiving the graded item.

### **Official Purdue University Student Policies**

<u>Student Expectations</u>: This is a 4 credit hour course, and it is expected that each student will spend 9 hours each week, including class time, on homework assignments, studying and reading the course textbook.

Student Conduct and Academic Integrity: University policy states that it is the responsibility of all students to attend all class sessions. Each student is expected to come to class on time and not disrupt the class. Each student is expected to follow Purdue's codes of student conduct and behave in a professional manner (https://www.purdue.edu/odos/academic-integrity). The rights of students in violation of the code of conduct are outlined. Each student is expected to exhibit consideration and respect towards the other students, the graders, the teaching assistants (TAs), and the faculty. Each student is expected to exhibit a positive attitude. Your conduct will be a factor in awarding grades to students between two letter grades.

Purdue University's student conduct policy specifically addresses academic dishonesty and integrity (http://www.purdue.edu/odos/osrr/academicintegritybrochure.php). All incidents of academic dishonesty will be reported to the Dean of Students. **Such incidents include:** 

- i) possessing or accessing, in hardcopy or electronic form, the solution manual to the course text or to the exams,
- ii) claiming credit for work (either HW or exam work) that is not your own original work, and
- iii) enabling another student to create HW or exam work that is not their original work.

<u>Instructors' Commitment</u>: Your instructors will: 1) be courteous, punctual, well-organized, and prepared for lecture and other class activities; 2) answer questions clearly in class or arrange for detailed discussions out of class if in-class answers are not suitably clear; 3) be available during office hours or notify you beforehand if they are unable to keep them; 4) provide a suitable guest lecturer when they are traveling; and 5) grade uniformly and consistently to the posted guidelines. We strongly encourage you to discuss academic or personal questions with the course instructor during office hours or via email. These discussions need not be limited to ChE 34800 content.

<u>Use of Copyrighted Materials</u>: Among the materials that may be protected by copyright law are the lectures, notes, and other material presented in class or as part of the course. All materials presented by an instructor are protected by copyright unless the instructor has stated otherwise. Students enrolled in, and authorized visitors to, Purdue University courses are permitted to take notes, which they may use for individual/group study or for other non-commercial purposes reasonably arising from enrollment in the course or the University generally.

Notes taken in class are, however, generally considered to be "derivative works" of the instructor's presentations and materials, and they are thus subject to the instructor's copyright in such presentations and materials. No individual is permitted to sell or otherwise barter notes, either to other students or to any commercial concern, for a course without the express written permission of the course instructor.

<u>Accessibility and Accommodations</u>: Purdue strives to make learning experiences as accessible as possible. If you anticipate or experience physical or academic barriers based on disability, you are welcome to let Prof. Tackett know to discuss options. You are also encouraged to contact the Disability Resource Center at: drc@purdue.edu or by phone: 765-494-1247.

<u>Grief Absence Policy for Students</u>: Purdue recognizes that a time of bereavement is very difficult for a student. Purdue therefore provides the following rights to students facing the loss of a family member through the Grief Absence Policy for Students (GAPS). GAPS Policy: Students will be excused for funeral leave and given the opportunity to earn equivalent credit and to demonstrate evidence of meeting the learning outcomes for missed assignments or assessments in the event of the death of a member of the student's family.

Please visit the University's website for additional information: <a href="http://www.purdue.edu/studentregulations/regulations/regulations">http://www.purdue.edu/studentregulations/regu

<u>Mental Health Statement</u>: If you find yourself beginning to feel some stress, anxiety and/or feeling slightly overwhelmed, try WellTrack, <a href="https://purdue.welltrack.com/">https://purdue.welltrack.com/</a>. Sign in and find information and tools at your fingertips, available to you at any time.

If you need support and information about options and resources, please see the Office of the Dean of Students, <a href="http://www.purdue.edu/odos">http://www.purdue.edu/odos</a>, for drop-in hours (M-F, 8am-5pm).

If you are struggling and need mental health services, Purdue University is committed to advancing the mental health and well-being of its students. If you or someone you know is feeling

overwhelmed, depressed, and/or in need of mental health support, services are available. For help, such individuals should contact Counseling and Psychological Services (CAPS) at (765)494-6995 and <a href="http://www.purdue.edu/caps/">http://www.purdue.edu/caps/</a> during and after hours, on weekends and holidays, or by going to the CAPS office of the second floor of the Purdue University Student Health Center (PUSH) during business hours.

<u>Violent behavior policy:</u> Purdue is committed to providing a safe and secure campus environment for members of the university community. Purdue strives to create an educational environment for students and a work environment for employees that promote educational and career goals. Violent Behavior impedes such goals. Therefore, Violent Behavior is prohibited in or on any University Facility or while participating in any university activity.

Please visit the University's website for additional information: <a href="http://www.purdue.edu/policies/facilities-safety/iva3.html">http://www.purdue.edu/policies/facilities-safety/iva3.html</a>

**Nondiscrimination Statement**: Purdue is committed to maintaining a community which recognizes and values the inherent worth and dignity of every person; fosters tolerance, sensitivity, understanding, and mutual respect among its members; and encourages each individual to strive to reach their own potential. In pursuit of its goal of academic excellence, the University seeks to develop and nurture diversity. The University believes that diversity among its many members strengthens the institution, stimulates creativity, promotes the exchange of ideas, and enriches campus life.

Purdue views, evaluates, and treats all persons in any University related activity or circumstance in which they may be involved, solely as individuals on the basis of their own personal abilities, qualifications, and other relevant characteristics.

Purdue prohibits discrimination against any member of the University community on the basis of race, religion, color, sex, age, national origin or ancestry, genetic information, marital status, parental status, sexual orientation, gender identity and expression, disability, or status as a veteran. The University will conduct its programs, services, and activities consistent with applicable federal, state, and local laws, regulations and orders and in conformance with the procedures and limitations as set forth in Purdue's Equal Opportunity, Equal Access and Affirmative Action policy which provides specific contractual rights and remedies. Additionally, the University promotes the full realization of equal employment opportunity for women, minorities, persons with disabilities and veterans through its affirmative action program.

Any question of interpretation regarding this Nondiscrimination Policy Statement shall be referred to the Vice President for Ethics and Compliance for final determination.

Please visit the University's website for additional information: <a href="http://www.purdue.edu/purdue/ea">http://www.purdue.edu/purdue/ea</a> eou statement.html

<u>Campus Emergency</u>: In the event of a major campus emergency, course requirements, deadlines and grading percentages are subject to changes that may be necessitated by a revised semester calendar or other circumstances beyond the instructor's control. Relevant changes to this course will be posted onto the course website or can be obtained by contacting the instructors or TAs via email or phone. <u>You are expected to read your @purdue.edu email on a frequent basis.</u>

### ChE 348 - Fall 2023 - <u>Tentative Course Schedule</u>

Assignment Due	Date	Topics
		Ch. 1: Definitions and mole balance equations
	Aug. 21	Lecture (Introduction to Course)
	Aug. 22	
	Aug. 23	Lecture
	Aug. 24	No Recitation (first week)
	Aug. 25	Lecture
		Ch. 2: Conversion and design equations
	Aug. 28	Lecture
	Aug. 29	
	Aug. 30	Lecture
HW 1	Aug. 31	Recitation
	Sep. 1	Recorded Lecture
		Ch. 3: Rate laws
	Sep. 4	No Class (Labor Day)
	Sep. 5	
	Sep. 6	Lecture
HW 2	Sep. 7	Recitation / pre-lab
	Sep. 8	Lecture
		Ch. 7: Experimental evaluation of rate parameters
	Sep. 11	Lecture
	Sep. 12	
	Sep. 13	Lecture
HW 3	Sep. 14	Lab #1
	Sep. 15	Lecture
		Ch. 4: Stoichiometry
	Sep. 18	Lecture
	Sep. 19	
	Sep. 20	Lecture
HW 4	Sep. 21	Recitation / pre-lab
	Sep. 22	Lecture

Assignment Due	Date	Topics
		Ch. 5: Isothermal reactor design
	Sep. 25	Lecture
	Sep. 26	
	Sep. 27	Recorded Lecture
Lab 1 report /HW 5	Sep. 28	Lab #2
	Sep. 29	Recorded Lecture
		Ch. 6: Semi-batch and membrane reactors
	Oct. 2	Lecture
	Oct. 3	
Exam 1	Oct. 4	Exam 1 (evening) Ch. 1,2,3,4,5,7
	Oct. 5	Recitation / pre-lab
	Oct. 6	Lecture
		Ch. 6: Semi-batch and membrane reactors
	Oct. 9	No Class (Fall Break)
	Oct. 10	
	Oct. 11	Lecture
Lab 2 report /HW 6	Oct. 12	Lab #3
	Oct. 13	Lecture
		Ch. 8: Multiple reactions
	Oct. 16	Lecture
	Oct. 17	
	Oct. 18	Lecture
HW 0 pt 1 /HW 7	Oct. 19	Recitation
	Oct. 20	Lecture
		Ch. 11: Energy balance and adiabatic reactors
	Oct. 23	Lecture
	Oct. 24	
Lab O man and	Oct. 25	Lecture
Lab 3 report /HW 8	Oct. 26	Recitation / pre-lab
	Oct. 27	Recorded Lecture

Assignment Due	Date	Topics
		Ch. 12: Steady-state reactors with heat exchange
	Oct. 30	Lecture
	Oct. 31	
	Nov. 1	Lecture
HW 9	Nov. 2	Lab #4
	Nov. 3	Lecture
		Ch. 13: Unsteady-state non-isothermal reactors
	Nov. 6	Recorded Lecture
	Nov. 7	
	Nov. 8	Lecture
HW 10	Nov. 9	Recitation
	Nov. 10	Lecture
		Ch. 10: Catalysis and catalytic reactors
Exam 2	Nov. 13	Exam 2 (evening) – Ch. 6, 8, 11, 12, (13)
	Nov. 14	
	Nov. 15	Lecture
Lab 4 report/ HW 11	Nov. 16	Recitation
	Nov. 17	Lecture
		Ch. 9: Mechanisms and bioreactors
	Nov. 20	Lecture
	Nov. 21	
	Nov. 22	No Class (Thanksgiving Break)
	Nov. 23	No Recitation (Thanksgiving Break)
	Nov. 24	No Class (Thanksgiving Break)
		Ch. 9 / Ch. 14: Mass transfer in reactors
	Nov. 27	Lecture
	Nov. 28	
	Nov. 29	Lecture
HW 12	Nov. 30	Recitation
	Dec. 1	Lecture

Assignment Due	Date	Topics
		Ch. 15 Diffusion and reaction
	Dec. 4	Lecture
	Dec. 5	
	Dec. 6	Lecture
	Dec. 7	Recitation
HW 0 pt 2 / Take-home project	Dec. 8	Lecture

Exam 3/ Final	TBD	Ch 1-15
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## CHE 540: Transport Phenomena

Instructors:	Prof. Vivek Narsimhan Room FRNY 1029B Phone: 765-494-4281 Email: vnarsim@purdue.edu
TA	Aaditya Joshi Room FRNY 3007 Email: joshi131@purdue.edu
Lectures:	Tues, Thurs 9:00 – 10:15 AM FRNY G124
Office Hours:	Prof. Narsimhan: Thurs 10:00 – 11:00 AM, FRNY 1029B or by email  Aaditya: Thurs: 4:30-5:30 PM, FRNY B124
Recitation (optional)	Aaditya: every two weeks (schedule to be decided)

### **Course Goals**

Develop a sound fundamental understanding of fluid mechanics, heat transfer, and mass transfer through theoretical/quantitative analysis. Use balance laws and dimensionless numbers to set up physical problems and simplify to underlying physics. Apply the concepts to solve problems of practical importance in chemical engineering and allied fields. Integrate the concepts of momentum, heat and mass transfer to acquire an understanding of the interrelation of these physical phenomena.

#### Textbook:

The following textbooks will be used for the class

- <u>Primary textbook:</u> *Introductory Transport Phenomena,* by R.B. Bird, W.E. Stewart, E.N. Lightfoot, and D.J. Klingenberg
- <u>Secondary textbook:</u> Analysis of Transport Phenomena, 2<sup>nd</sup> Ed, by William M. Deen, Chapters 1-12

### **Website for Course Information:**

http://purdue.brightspace.com

This course will use the Brightspace for syllabus, handouts, homework, and solutions. To login, use your university name and password. Please check the website regularly for assignments as paper copies will not be handed out in class. Generally, homework is due on Fridays, and homework will be posted a week before it is due. Recitation problems will be posted prior to recitation sessions, and you should bring a copy of the problems to recitation.

The course will also use Gradescope for submission of homework and to keep track of grades. This can be accessed through Brightspace.

### E-mail

Occasionally, important class announcements will be disseminated through the class e-mail list. It is your responsibility to regularly check your e-mail every day and to read the e-mails regarding CHE 540 to receive important class information. If you e-mail Profs. Narsimhan with questions or a request to make an appointment, please allow a minimum of 24 hours for a response during the week (or a response by Tuesday morning if the e-mail is sent on the weekend).

### **Grading Policy:**

Homework (~9-10 total) 30%

Two midterms 40% (20% each)

Final exam 30%

Total 100%

Homework will be due on Fridays at the beginning of lecture. Unless specified by the instructor, the latest a homework can be turned in is two days past the due date (Sun 1:30 PM). Late homework will lose 20% off its maximum score for each day tardy. Homework after Sun 1:30 PM will count as a zero. Students will be allowed to drop one homework from their final grade.

### **Makeup lectures:**

There are currently no makeup lectures scheduled for this class. If makeup does need to be schedule, it will be done so at a future date.

#### **Exam Times**

There will be two midterms in this class. The first midterm will be in mid Feb, and the second midterm will be at the end of March. The dates and location will be announced at least three weeks before the exam.

The final exam will happen in the last week of the semester (May 2-7). The final exam schedule is to be determined.

Any student who cannot take an exam as scheduled (e.g., due to conflicts with another exam) *must* make special arrangements by sending Profs. Narsimhan an e-mail at least two weeks *before* the exam. Individual make-up exams *will not* be given. In cases of extenuating circumstances or extreme duress (e.g., hospitalization), please provide documentation to Profs. Narsimhan, and if possible, speak to us *before* the exam takes place. A single comprehensive make-up exam (available only for students who miss a test) will be administered during finals period. *This will be the only make-up exam available*.

### **Syllabus**

Part I: Heat and mass transfer (~6 weeks). Chapters 9-11, 17-19 in BSL-K, Chapters 1-5 in Deen

Lecture 1	Introduction to vector calculus – vectors, tensors, and divergence
Lecture 1	theorem (Deen Appendix)
	theorem (Seem Appendix)
	Balance laws for heat and mass transfer – introduction to fluxes ((BSL-
	K Ch 0, BSL-K Ch 9, BSL-K Ch 17, Deen Ch 1, Deen Ch 2)
Lecture 2	Introduction to Fourier's/Fick's law.
	Boundary conditions and heat transfer coefficients. (BSL-K Ch 0, BSL-K
	Ch 9, BSL-K Ch 17, Deen Ch 1, Deen Ch 2)
Lecture 3	Heat transfer in composite solids series and parallel resistances
	(BSL-K Ch 10.3)
	Introduction to Biot number. Reduction in dimensionality ad scaling
	(BSL-K Ch 10.2, Deen Ch 3.4.1)
Lecture 4	Finish up discussion on Biot number (BSL-K Ch 10.2, Deen Ch 3.4.1)
	Heat transfer in fins (BSK-K Ch 10.5)
Lecture 5	1D problems – reaction diffusion systems. Introduction to Damkoler
	number, spherical catalyst (BSL-K Ch 18.5, Deen Ch 3.2)
	Introduction to diffusion in gases (pseudo-binary approximation) (BSL-
	K Ch 18.6)
Lecture 6	Continue discussion on diffusion in gases (BSL-K Ch 18.6)
	Dec. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1.
	Pseudo steady-state approx. (BSL-K Ch18.7, BSL-K Ex. 18.4-1, BSL-K Ex.
Lookiino 7	18.6-1, Deen Ch 3.5)
Lecture 7	Continue discussion of pseudo steady state
Lecture 8-9	Similarity solutions for heat/mass transfer problems (BSL-K Ch 11.5,
	BSL-K Ch 18.8, Deen Ch 4.2)
Lectures 10	Review (if necessary)
	EXAM 1
Lectures 11-12	Separation of variables (BSL-K Ex 11.5-2, Deen Ch 5)

**Part II: Fluid mechanics (~5 weeks).** Chapters 1-6 in BSL-K, Chapters 6-7, 9 in Deen

Lecture 13	Introduction to tensors
	Cauchy momentum equations (BSL-K Ch 3.2, Deen Ch 6.2-6.3)
Lecture 14	Continuation of Cauchy momentum equations
	Introduction to stress tensor (BSL-K Ch 1, BSL-K Ch 3.6, Deen Ch 6.4)
Lecture 15	Continuation of stress tensor
	Hydrostatics (BSL-K Ch 2.7, Deen Ch 6.6)

Lecture 16-17	Boundary conditions for flow and surface tension (BSL-K Ch 2.1) Example problem surface tension
Lecture 18	Unidirectional flows: Poiseuille and Couette flows (BSL-K Ch2.3, BSL-K Ch 2.5, Deen Ch 6)
	Introduction to lubrication flows
Lecture 19-20	Lubrication theory and examples (rigid surfaces and free surfaces) (Deen Ch 7.6)
Lecture 21	Inviscid flow – derivation of Bernoulli's equation (BSL-K Ch 3.3, BSL-K Ch 7.4, Deen Ch 9.1-9.2)
Lecture 22	Review (if necessary)
	EXAM 2

# Part III: Applications (~3 weeks). Chapters 7, 14-15, 21-23 in BSL-K, Chapter 9 in Deen

Lecture 23	Momentum boundary layers (concepts). Scaling of boundary layer (BSL-K Ch 3.8, Deen Ch 8)
	Introduction to friction factors (BSL-K Ch 6)
Lecture 24-25	Convective heat and mass transfer. Introduction, boundary layer,
	Sherwood/Nusselt numbers (BSL-K Ch 19.4, BSL-K Ch 20.4, BSL-K Ch
	22.1, Deen Ch 9, Deen Ch 10)
	Estimating heat and mass transfer coefficients via correlations
Lectures 26-27	Macroscopic mass and energy balances (BSL-K Ch 7, Ch 11)
Lecture 28	Example of macroscopic balance: heat exchangers (BSL-K Ex 15.3-1,
	BSL-K Ex 15.4-1)
Lecture 29	Example of macroscopic balance: dialysis, or friction loss in pipes, etc.
	(BSL-K Ex 23.1-3)
Lectures 30	Final exam review

### Accommodating students with disabilities:

Purdue University strives to make learning experiences as accessible as possible. If you anticipate or experience physical or academic barriers based on disability, you are welcome to let me know so that we can discuss options. You are also encouraged to contact the Disability Resource Center at <a href="mailto:drc@purdue.edu">drc@purdue.edu</a> or by phone: 765-494-1247.

In addition to the University policy, the Davidson School of Chemical Engineering has established procedures for students seeking accommodations. These can be found online at the ChE Undergrad Office website. Only those accommodation requests that conform to both University and ChE policy guidelines will be implemented.

### **Academic Dishonesty:**

Academic dishonesty will not be tolerated in any form in this course. Specifically, Purdue prohibits "dishonesty in connection with any University activity. Cheating, plagiarism, or knowingly furnishing false information to the University are examples of dishonesty." [Section B-2-a, Code of Student Conduct] Furthermore, the University Senate has stipulated that "the commitment of acts of cheating, lying, and deceit in any of their diverse forms (such as the use of substitutes for taking examinations, the use of illegal cribs, plagiarism, and copying during examinations) is dishonest and must not be tolerated. Moreover, knowingly to aid and abet, directly or indirectly, other parties in committing dishonest acts is in itself dishonest." [University Senate Document 72-18, December 15, 1972] All incidents of academic dishonesty will be reported to the Dean of Students. Such incidents include: i) possessing or accessing, in hardcopy or electronic form, the solution manual to the course text, or to the exams, ii) claiming credit for work that is not your own original work, and iii) enabling other students to create work that is not their original work. The punishment for a first offense on a homework assignment is a grade of zero for the entire work and the punishment for a second offense is an F grade for the class. The punishment for any offense for an exam is an F grade for the class.

#### **Conduct:**

University policy states that it is the responsibility of all students to attend all class sessions (http://www.purdue.edu/studentregulations/regulations\_procedures/classes.html). Each student is expected to come to class on time and not disrupt the class. Each student is also expected to follow Purdue's codes of student conduct"

### (http://www.purdue.edu/studentregulations/student conduct/regulations.html)

and behave in a professional manner. The rights of students in violation of the code of conduct are outlined. Each student is expected to exhibit consideration and respect towards the other students, the graders, the teaching assistants (TAs), and the faculty member. Each student is expected to exhibit a positive attitude. Your conduct will be a factor in awarding grades to students between two letter grades. Purdue University's student conduct policy specifically addresses academic dishonesty.

### **Violent Behavior Policy:**

Purdue University is committed to providing a safe and secure campus environment for members of the University community. Purdue strives to create an educational environment for students and a work environment for employees that promote educational and career goals. Violent behavior impedes such goals. Therefore, violent behavior is prohibited in or on any University Facility or while participating in any University activity.

#### Nondiscrimination:

Purdue University is committed to maintaining a community which recognizes and values the inherent worth and dignity of every person; fosters tolerance, sensitivity, understanding, and mutual respect among its members; and encourages each individual to strive to reach his or her own potential. In pursuit of its goal of academic excellence, the University seeks to develop and nurture diversity. The University believes that diversity among its many members strengthens the institution, stimulates creativity, promotes the exchange of ideas, and enriches campus life. Purdue University prohibits discrimination

against any member of the University community on the basis of race, religion, color, sex, age, national origin or ancestry, genetic information, marital status, parental status, sexual orientation, gender identity and expression, disability, or status as a veteran. The University will conduct its programs, services and activities consistent with applicable federal, state and local laws, regulations and orders and in conformance with the procedures and limitations as set forth in Executive Memorandum No. D-1, which provides specific contractual rights and remedies. Any student who believes they have been discriminated against may visit www.purdue.edu/report-hate to submit a complaint to the Office of Institutional Equity. Information may be reported anonymously.

### **Emergency Preparedness:**

Purdue University is a very safe campus and there is a low probability that a serious incident will occur here at Purdue. However, it is important to emphasize the emergency procedures for evacuation and shelter-in-place incidents. Preparedness will be critical if an unexpected event is to occur. Emergency preparedness is your personal responsibility. Purdue University is actively preparing for natural disasters or human-caused incidents with the ultimate goal of maintaining a safe and secure campus. The following is a review of the emergency procedures at Purdue University.

- 1. For any emergency call 911.
- 2. There are nearly 300 Emergency Telephone Systems throughout campus that connect directly to the Purdue Police Department (PUPD). If you feel threatened or need help, push the button and you will be connected to the PUPD.
- 3. If there is a fire alarm, we will immediately evacuate the building and proceed to in front of the MSEE building. Do not use the elevator.
- 4. If there is a Shelter-in-Place requirement for a tornado warning, we will shelter in the lowest level of this building away from windows and doors. This location is between FRNY G140 and FRNY B124.
- 5. If there is a Shelter-in-Place requirement for a hazardous materials release, we will shelter in the classroom shutting any open doors and windows.
- 6. If there is a Shelter-in-Place requirement for a civil disturbance, we will shelter in a room that is securable preferably without windows. This location is FRNY 2182.



## **ChE 554: Smart Manufacturing in the Process Industries**

**Course Information** 

Instructor(s) Contact Information

**Course Description** 

**Learning Resources, Technology & Texts** 

**Learning Outcomes** 

Assignments

**Grading Scale** 

Course Schedule

**Academic Integrity** 

**Nondiscrimination Statement** 

**Accessibility** 

Mental Health/Wellness Statement

**Basic Needs Security** 

**Emergency Preparation** 

### Course Information

- ChE 554: Smart Manufacturing in the Process Industries
- CRN: 27600/28664/28663
- Instructional Modality: Asynchronous-Online
- Meeting day(s) and time(s). This course starts on August 21 and runs until December 9. However, there are no formal class meeting times since this is considered an Asynchronous-Online course. This means that you will independently watch the recorded lectures in Brightspace to complete assignments.
- Course credit hours: 3
- Prerequisites (if any): A basic understanding of Python Programming

### **Instructors Contact Information**

- Professor J. Pekny (Course Coordinator)
  - Email: pekny@purdue.eduOffice Location: FRNYOffice Number: G027C
- Professor G V Reklaitis
  - Email: reklaiti@purdue.eduOffice Location: FRNYOffice Number: G027B
- Professor Z. Nagy
  - Email: znagy@purdue.edu
     Office Location: FRNY
     Office Number: G027D
- Student Consultation hours, times, and location: Each week, a different instructor will present content, asynchronously. Please email the instructor in question for specific questions about the content they presented. For administrative questions including grades, and other please email Dr. Pekny, the course coordinator. You should hear a response from your instructors within 24-48 hours in most cases.

### **Course Description**

This course surveys the tools and techniques which are relevant to support the multiple levels of technical decisions that arise in modern integrated operation of manufacturing resources in the chemical, petrochemical and pharmaceutical industries. The real time generation and sharing of associated data and knowledge via relevant IT methodology and the effective use of this information in the various levels of the process operations management hierarchy are currently termed **Industry 4.0** (Europe) and **Smart Manufacturing** (US). The topics covered in the course span all the technical components and decision levels in the operations decision hierarchy. Topics include the role of on-line and at-line process measurements, elements of sensor network design, information systems to support process operations, plant data reconciliation, detection and diagnosis of process faults, condition-based monitoring of plant assets, plant wide control, real time process optimization, production planning and scheduling, and supply chain management. Each topic will be addressed by first summarizing the basic role and scope of that component, then discussing the elements of the decision problem, and outlining some representative tools available to address that decision problem. Each major topic will include a lecture given by an industrial practitioner who will offer a perspective on the state of industrial practice.

### **Learning Resources, Technology & Texts**

### There is NO required textbook for this course.

o There will be readings available within Brightspace.

#### Software

- MatLab (which can be accessed via ECN). For more information about accessing Matlab, click <u>here.</u>
- We will also be analyzing data using "Anaconda," (a popular Python distribution), click <a href="here">here</a> to learn more about how to download it and get started.

### Hardware requirements

 A laptop that can connect to the internet and run the <u>Microsoft Office Suite</u> ( available free to all Purdue Students)

### • Brightspace learning management system

O Access the course via Purdue's Brightspace learning management system. Begin with the Start Here tab, which describes how the course Brightspace is organized. It is strongly suggested that you explore and become familiar not only with the site navigation but with the content and resources available for this course. See the Student Services widget on the campus homepage for resources such as Technology Help, Academic Help, Campus Resources, and Protect Purdue.

### **Learning Outcomes**

- 1. Explain the key decisions that are made at each level of the operational hierarchy of an integrated process system.
- 2. Define what the various types of manufacturing and enterprise data are, how they are generated and managed and what their functions are in supporting these decisions.
- 3. Explain the role of models in supporting the decisions made at each level of the operational hierarchy.
- 4. Evaluate and improve a plant wide control system for a given manufacturing system.
- 5. Identify condition-based monitoring of a manufacturing system, how it is performed and what its outcomes should be.
- 6. Explain the nature and role of planning and scheduling models and tools as applied at the plant and supply chain levels.

### **Assignments**

Assignment	Description	% Of Grade
HW/Labs	The goal of these labs is to give you real-world problems to solve using the information presented. More information about each of the homework/labs can be found in Brightspace.	60%
Final Project	While we encourage you to choose the "scope" of your project based on your interest level towards specific topics presented in the course and the application to your current or future career, your topic still needs to be approved.	40%
L		Total: 100%

### **Grading Scale**

In this class grades reflect the sum of your achievement throughout the semester. You will accumulate points as described in the assignments portion above, with each assignment graded according to a rubric. At the end of the semester, final grades will be calculated by adding the total points earned and translating those numbers (out of the maximum available) into the following letters (there will be no partial points or rounding).

A: 93.5%-100%
A-: 89.5%-93.49%
B+: 86.5%-89.49%
B-: 79.5%-82.49%
C+: 76.5%-79.49%
C-: 69.5%-72.49%
D+: 66.5%-69.49%
D-: 59.5%-62.49%

Academic Integrity

F: 49.4%-below

Academic integrity is one of the highest values that Purdue University holds. Individuals are encouraged to alert university officials to potential breaches of this value by either emailing integrity@purdue.edu or by calling 765-494-8778. While information may be submitted anonymously, the more information is submitted the greater the opportunity for the university to investigate the concern. More details are available on our course Brightspace table of contents, under University Policies.

### **Nondiscrimination Statement**

A hyperlink to Purdue's full Nondiscrimination Policy Statement is included in our course Brightspace under University Policies.

### Accessibility

Purdue University is committed to making learning experiences accessible. If you anticipate or experience physical or academic barriers based on disability, you are welcome to contact the course coordinator to discuss options. You are also encouraged to contact the Disability Resource Center at: <a href="mailto:drc@purdue.edu">drc@purdue.edu</a> or by phone: 765-494-1247.

# **Course Schedule**

Week	Topics	Assignments
Week 1	Introduction to Smart Manufacturing	
Week 2	Sensors and Plant Data Reconciliation	HW/Lab 1 - Data Reconciliation
Week 3	Error Detection and Information Systems	
Week 4	Statistical Methods and Monitoring/Diagnosis Applications	HW/Lab 1
Week 5	PLS Models and Applications and Review of Diagnostic Methods	HW/Lab 2 - Process Analytics using Multivariate Methods
Week 6	Condition Based Monitoring	
Week 7	ML and Al Models	
Week 8	Data Analytics	
Week 9	Optimization	
Week 10	State Estimation	HW/Lab 3 - Optimization
Week 11	Plant Wide Control	
Week 12	Scheduling and Planning Introduction	HW/Lab 4 - Plant Wide Control
Week 13	Scheduling and Planning Methods	
Week 14	Industrial Application	HW/Lab 5 - Scheduling and Planning
Week 15	Supply Chain Management	
Week 16	Final Group Projects	Final Presentation

<sup>\*</sup> Schedule and assignments subject to change. Any changes will be posted in the learning management system.

# **Mental Health/Wellness Statement**

If you find yourself beginning to feel some stress, anxiety and/or feeling slightly overwhelmed, try <u>WellTrack</u>. Sign in and find information and tools at your fingertips, available to you at any time.

**If you need support and information about options and resources**, please contact or see the <u>Office of the Dean of Students</u>. Call 765-494-1747. Hours of operation are M-F, 8 am- 5 pm.

If you find yourself struggling to find a healthy balance between academics, social life, stress, etc. sign up for free one-on-one virtual or in-person sessions with a <u>Purdue Wellness Coach at RecWell</u>. Student coaches can help you navigate through barriers and challenges toward your goals throughout the semester. Sign up is completely free and can be done on BoilerConnect. If you have any questions, please contact Purdue Wellness at <u>evans240@purdue.edu</u>.

If you're struggling and need mental health services: Purdue University is committed to advancing the mental health and well-being of its students. If you or someone you know is feeling overwhelmed, depressed, and/or in need of mental health support, services are available. For help, such individuals should contact <a href="Counseling and Psychological Services">Counseling and Psychological Services</a> (CAPS) at 765-494-6995 during and after hours, on weekends and holidays, or by going to the CAPS office on the second floor of the Purdue University Student Health Center (PUSH) during business hours.

# **Basic Needs Security**

Any student who faces challenges securing their food or housing and believes this may affect their performance in the course is urged to contact the Dean of Students for support. There is no appointment needed and Student Support Services is available to serve students 8 a.m.-5 p.m. Monday through Friday. Considering the significant disruptions caused by the current global crisis as it related to COVID-19, students may submit requests for emergency assistance from the Critical Needs Fund

# **Emergency Preparation**

In the event of a major campus emergency, course requirements, deadlines and grading percentages are subject to changes that may be necessitated by a revised semester calendar or other circumstances beyond the instructor's control. Relevant changes to this course will be posted onto the course website or can be obtained by contacting the instructors or TAs via email or phone. You are expected to read your @purdue.edu email on a frequent basis.



# Spring 2024 CHE 597

# **Advanced Solar Energy Conversion**

T/TH 10:30 AM - 11:45 AM

Instructor: Dr. Rakesh Agrawal

Office: FRNY, RM 3053D Email: <u>agrawalr@purdue.edu</u>

### Melissa LaGuire

NRT Program Coordinator Email: mlaguire@purdue.edu

Course Objective: To introduce working principles of solar cells to engineers who are not that familiar with the solid-state electronic devices. The students will learn (1) what makes a good material for harnessing solar energy, (2) how to use these materials to design efficient solar cells, and (3) details about solar spectrum and thermodynamic limits of various solar cell structures in converting solar energy to electricity. One benefit of this course is that the principles learned are applicable to a wide array of electronic and optoelectronic devices being manufactured by ever increasing companies in the arena of renewable energy, electronic chips and devices.

**Recommended Books:** There is no textbook for this course, but following are recommended as references.

- 1. The Physics of Solar Cells, by Jenny Nelson, Imperial College Press. ISBN: 1-86094-349-7 (pbk).
- 2. Physics of Solar Cells From Principles to New Concepts, by Peter Würfel, Wiley VCH. ISBN: 3-527-40428-7.
- 3. Principles Of Solar Cells: Connecting Perspectives On Device, System, Reliability, And Data Science, M. Ashraf Alam and M. Ryyan Khan, WSPC, ISBN-10: 9811233020

Both books are available in the Reserve Section of the Potter Engineering Library. Although, not essential, it may like to own one of the books, preferably the one by Nelson or Alam.

**Homework and Exams:** The following weightages assigned to homework and exams:

Homework 30% Exam 1 35% Exam 2 35%

In order to master the course, it is essential that you do all the home works in a timely manner.

# **Homework Policy:**

For the first homework that is less than one day late, 30% mark will be deducted. For the second homework that is less than one day late, 50% mark will be deducted. For any other late homework, no credit will be given.

# **Important Dates:**

Exam 1 – Thursday 22<sup>nd</sup> February

Exam 2 – Thursday 18<sup>th</sup> April

All the exams will be during the lecture period. Final grading for the course will be done using letter grades A, B, C, D and F.

#### **Makeup Classes:**

Please be aware there is a possibility of makeup classes for this course. The dates and times will be announced in advance if necessary.

<u>Bright Space page</u>: You can access the course via Brightspace. It is strongly suggested that you explore and become familiar not only with the site navigation, but with content and resources available for this course.

# **Guidelines for Academic Integrity:**

All students will conduct according to Purdue's Honor Pledge (<a href="https://www.purdue.edu/provost/teachinglearning/honor-pledge.html">https://www.purdue.edu/provost/teachinglearning/honor-pledge.html</a>): "As a boilermaker pursuing academic excellence, I pledge to be honest and true in all that I do. Accountable together - we are Purdue." Every student will sign this pledge in their first homework assignment, each exam and project report.

While Students are encouraged to discuss homework problems with each other, the submitted work must be work of the individual and no copying is allowed.

We will enforce the penalty if a student is caught cheating as proposed by Purdue:

"Incidents of academic misconduct in this course will be addressed by the course instructor and referred to the Office of Student Rights and Responsibilities (OSRR) for review at the university level. Any violation of course policies as it relates to academic integrity will result minimally in a failing or zero grade for that particular assignment, and at the instructor's discretion may result in a failing grade for the course. In addition, all incidents of academic misconduct will be forwarded to OSRR, where university penalties, including removal from the university, may be considered."

# **Expected Conduct in the Class:**

Avoid being late to the lectures (even though it is remote).

Be attentive during lectures.

It is encouraged to ask clarifying questions during lecture.

**Covered Topics:** The following major topics will be covered in the lectures:

- 1. Solar Radiation
  - a. Thermal radiation from a black body Planck's law

- b. Thermal radiation from Sun on an area on Earth
- c. Solar radiation through Earth's atmosphere
- 2. Thermodynamic Efficiency of Solar Energy Recovery as work
- 3. Solar Thermal Power
  - a. Concentrating Solar Power
  - b. Advantages and disadvantages for solar thermal
- 4. General Introduction to Solid State Solar Cells
  - a. Concept of a diode
  - b. Current-voltage, relationship in a solar cell short circuit current, open circuit current, open circuit voltage, fill factor series and shunt resistance.
- 5. Electrons and Holes in Semiconductors
  - a. Brief Review of the Physical Structure of Solids
  - b. Energy bands in Solids
  - c. Brief Introduction to quantum mechanics
  - d. Density of energy states for free electrons in a box
  - e. Density states for a 3D body
  - f. Fermi-Dirac distribution function (Fermi function)
  - g. Electron in a periodic potential Origin of band diagrams
  - h. Concept of holes in valence band
- 6. Intrinsic and Extrinsic Semiconductors
  - a. Electron and hole concentrations in intrinsic semiconductors
  - b. n & p type extrinsic semiconductors
- 7. Charge transport in a semiconductor
  - a. Charge neutrality relationship
  - b. Mobility of electron and holes in an electric field drift current
  - c. Diffusion current
  - d. Einstein relationship relating diffusion coefficient and mobility
  - e. Nonequilibrium semiconductor quasiFermi levels
  - f. Charge separation and collection charge separation under illumination
- 8. Generation and recombination in semiconductors
- 9. p-n junction in the absence of light
  - a. Internal electric field in a homo p-n junction
  - b. Calculation of built in potential
  - c. Width of space charge region under forward or reverse bias
  - d. Transport equations for the p-n junction
  - e. Saturation current and diode factor
  - f. Performance of thin p-n diodes
- 10. Solar Cells p-n junction under illumination

- a. Governing equations for p-n junction under light illumination
- b. Dimensionless parameters for assessing solar cell performance
- 11. Different Solar Cell Structures Advantages and Limitations
  - a. Silicon solar cells
  - b. Thin film inorganic solar cells CdTe/CdS, CIGS/CdS etc.
  - c. Organic solar cells
  - d. Solar modules and the balance of systems
- 12. General Discussion on the Future of Solar Cells
  - a. Interdisciplinary nature of solar cells
  - b. Cost and efficiency issues

#### Additional Information:

In the event of a major campus emergency, course requirements, deadlines and grading percentages are subject to changes that may be necessitated by a revised semester calendar or other circumstances beyond the instructor's control..

Purdue University strives to make learning experiences as accessible as possible. If you anticipate or experience physical or academic barriers based on disability, you are welcome to let me know so that we can discuss options. You are also encouraged to contact the Disability Resource Center at drc@purdue.edu or by phone: 765-494-1247.

In addition to the University policy, the Davidson School of Chemical Engineering has established procedures for students seeking accommodations. These can be found online at the ChE Undergrad Office website. Only those accommodation requests that conform to both University and ChE policy guidelines will be implemented.

# Spring 2024 CISTAR course: Energy Transition to a Sustainable Future

The CISTAR course – Energy Transition to a Sustainable Future – will be offered virtually with four CISTAR Universities in the Spring of 2022. It will be offered as a 3 credit (semester basis) hr course (or equivalent). The course is targeted at entering graduate students, but advanced undergraduates may also enroll in the class.

#### **Instructors:**

Joan Brennecke University of Texas at Austin <u>jfb@che.utexas.edu</u>
Abhaya Datye University of New Mexico <u>datye@unm.edu</u>

Jeff Miller Purdue University <u>mill1194@purdue.edu</u>

Ruilan Guo University of Notre Dame rguo@nd.edu

#### Time:

MW 4:30-5:45p Eastern (PU and ND)

MW 3:30-4:45p Central (UTA)

MW 2:30-3:45p Mountain (UNM)

# **Short description:**

A survey course on all aspects of the transition from fossil fuels to more sustainable energy resources. This will include an understanding of 1) current energy production and use, 2) the importance of light hydrocarbons as a bridge to a net-zero carbon economy, 3) the environmental implications of energy production and storage, 4) carbon capture, sequestration and conversion, 5) the role that electrification plays in the transition, and 6) sources of low-CO<sub>2</sub> footprint energy necessary to achieve a sustainable energy future.

### **Learning Objectives:**

- 1. Understand the historical, current and potential future roles that hydrocarbons play in the economy for energy, fuels, and materials.
- 2. Understand the environmental impact (environmental, health, legal, social) of various aspects of energy production and use.
- 3. Understand the methods for carbon capture, storage and conversion to meet future environmental CO<sub>2</sub> reductions.
- 4. Understand the options for decarbonization of energy production.

Class Schedule: We are currently confirming the guest lectures who we leading experts on these topics. At the end of the semesters, student teams (4 students each) will submit a written report and give a 20 min lecture on a topic of their choosing.

# \* Home Work:

- HW 1 Students select projects of most interest
- HW 2 Team formation and information exchange
- HW 3 Literature Citations due (minimum 15)
- HW 4 Outline of report content due
- HW 5 Draft Report due (10 pages)

1 week after draft report: Draft report feedback

# Grading

• Exam (40%):

Multiple choice

• Homework/Class Participation (10%)

Report outline, draft report

- Written Final Project Report (25%): 10 pages
- Oral Final Project Report (25%): 25 min + 12 min Q&A

# Purdue University CHE 59700: Electrochemistry and Electrochemical Engineering – 3 credits

Spring 2023 (Final version available at start of class)

Time/Location: Tues/Thurs

10:30AM FRNY 1043

Synchronous, In-person (recordings available via Boilercast)

**Instructor:** Brian Tackett

Assistant Professor Chemical Engineering

Email: <u>bmtacket@purdue.edu</u>

**Office:** FRNY 2158 **Phone:** 7654967235

Office Hours: Weds 10:00 AM

FRNY 2158

Course
Description and
Learning
Outcomes:

This course will provide students with a technical working knowledge of electrochemical phenomena to prepare them for the wide range of electron-driven processes emerging in industry and research.

By the end of the course, students will be able to:

- 1. Describe the components of an electrochemical reaction system and qualitatively explain how it works
- 2. Formulate basic thermodynamic, kinetic, and mass transport relationships of electrochemical reaction systems
- 3. Apply these formulations to calculate required operating parameters (energy/overpotential, current density, etc.) to meet specified electrochemical production
- 4. Comprehend and select appropriate electroanalytical techniques to answer research questions about electrochemical systems

**Required Text:** 

West, A. C. *Electrochemistry and Electrochemical Engineering. An Introduction*; 2012.

Supplemental Texts:

- Bard, A. J.; Faulkner, L. R. *Electrochemical Methods: Fundamentals and Applications*; 2<sup>nd</sup> ed. 2001, or 3<sup>rd</sup> ed. 2022.
   See also: "Electroanalytical Chemistry Lectures" by D Wipf (Prof. David O. Wipf) on YouTube
- Prentice, G. Electrochemical Engineering Principles; 1991
- Newman, J.; Thomas-Alyea, K. E. *Electrochemical Systems*; 3<sup>rd</sup> ed. 2004.
- Bockris, J. O'M.; Reddy, A. K. N. Modern Electrochemistry, Vol 1, Vol 2a, Vol 2b; 2<sup>nd</sup> ed 2000. (available in pdf online from Springer).
- Pletcher, D. A First Course in Electrode Processes: 2<sup>nd</sup> ed. 2009.

Technology

Regiurement: MS Office

# Purdue University CHE 597 Industrial Chemical Technology Fall 2023, Tue-Thu 1:30-2:45, HAMP 2102

Instructor: Jeff Siirola, FRNY 1029A, 6-2125, jsiirola@purdue.edu or jjsiirola@gmail.com

Office Hours: Almost anytime; best to make appointment by email

### **Course Description:**

This course traces the historical development of the chemical and related process industries and describes the principal products that are made and the evolution of the raw materials, chemistries, and processes by which they have been made. The scope includes natural products, inorganics, fuels, and commodity and specialty organics. The course also covers topics of current interest including the impacts of modern catalysis, digital computation, and systems engineering on process technology, issues of sustainability, resource conservation, environmental responsibility, product stewardship, and carbon management, and the likely impacts of recently more abundant and less expensive shale gas and oil on the chemical industry.

#### **Course Content:**

History and structure of the chemical and allied process industries (1 week)

Natural Products (animal and vegetable products; wood derivatives) (1 week)

Inorganics (dehydration (calcining), reduction (smelting), bases and acids, commodities) (2 weeks)

Fuels (fossil, petroleum refining, synthetic and biofuels) (1.5 weeks)

Organics (wood and coal derivatives, basic building blocks, commodity intermediates and solvents, commodity monomers and polymers, plastics fibers and coatings, fine chemicals, biotechnology) (4 weeks)

Technical Impact Factors (catalysis, computers, innovation) (1.5 weeks)

Current Issues (environmental protection, health and safety, sustainability, carbon dioxide management, shale gas and oil) (3.5 weeks)

#### **Tentative course schedule (subject to change):**

munic course	senedure (subject to enunge).
Tue 22 Aug	Course introduction; scope of the chemical and allied process industries
Thu 24 Aug	Historical technology development (alchemy, chemistry, processes, unit
	operations, transport phenomena, process systems); historical milestones
	(brewing, soap, salt, smelting, soda ash, distillation, electrolysis, high
	pressure, continuous controlled processes)
Tue 29 Aug	Natural Products 1 - Animal and vegetable fiber, leather, oils, fats, waxes,
	gelatin, dairy products, food processing
Thu 31 Aug	Natural Products 2 - Pulp and paper, naval stores, resins, turpentine, rosin,
	rubber (Report 1 Due)
Tue 5 Sep	Inorganics 1 - Chemistry of dehydration/hydration: ceramic pottery, tile, and
	brick, glass, plaster, cement, mortar, and concrete
Thu 7 Sep	Inorganics 2 - Chemistry of reduction: ore smelting, iron and steel, silicon,
	copper, brass, bronze, aluminum

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Tue 12 Sep	Inorganics 3 - Bases and acids: soda ash, caustic soda, lime, mineral acids (nitric, sulfuric, phosphoric, hydrochloric)
Thu 14 Sep	Inorganics 4 - Commodity inorganics: water, hydrogen, oxygen, nitrogen,
	chlorine, fertilizers (ammonia, phosphates, potash), titanium dioxide,
	carbon black, carbon dioxide, phosgene, hydrogen peroxide (Report 2
	Due)
Tue 19 Sep	Fuels 1 - Wood, coal, petroleum (gasoline, diesel, jet fuel, fuel oil), LPG, natural gas
Thu 21 Sep	Fuels 2 - Natural gas processing, petroleum refining processes and products
Tue 26 Sep	Fuels 3 - Synthetic fuels: town gas, F-T, SNG, MTG, biofuels
Thu 28 Sep	Organics 1 - Wood and coal chemicals and materials (Report 3 Due)
Tue 3 Oct	Organics 2 - Basic building blocks: acetylene, olefins (ethylene, propylene,
m	butadiene) aromatics (BTX, Styrene), carbon monoxide
Thu 5 Oct	Organics 3 - Commodity intermediates and solvents: alcohols glycols and
T 100	phenols, aldehydes and ketones, acids, esters, ethers
Tue 10 Oct	No Class - Fall Break
Thu 14 Oct	Organics 4 - Commodity monomers and polymers (PE, PP, PS, PET, PC, SBR) (Report 4 Due)
Tue 17 Oct	Organics 5 - Adhesives, coatings, films, fibers, plastics (Report 4 Due)
Thu 19 Oct	Organics 6 - Fine chemicals: dyes pigments and cosmetics, flavors and
	fragrances, soap and detergents, explosives, agrichemicals,
	pharmaceuticals
Tue 24 Oct	Organics 6 continued
Thu 26 Oct	Organics 7 - Fermentation and biochemical processes; biotechnology (Report 5 Due)
Tue 31 Oct	Technical Impact Factor 1 - Homogeneous and heterogeneous catalysis
Thu 2 Nov	Technical Impact Factor 2 - Engineering and operational digital computation
Tue 7 Nov	Possible No Class -AIChE Meeting
Thu 9 Nov	Current Issues 1 - Environmental protection: air, wastewater, land; personnel protection: health and safety (Report 6 Due)
Tue 14 Nov	Current Issues 2 - Loss prevention and process safety
Thu 16Nov	Current Issues 3 - Sustainability: triple bottom line, life cycle analysis, industrial ecology, green chemistry and engineering
Tue 21 Nov	Possible No Class (Early Thanksgiving Break)
Thu 23 Nov	Thanksgiving
Tue 28 Nov	Current Issues 4 - Sustainability: population and economic growth, raw
	materials and energy demands
Thu 30 Nov	Current Issues 5 - Climate change
Tue 5 Dec	Current Issues 6 - Carbon dioxide management, capture, and sequestration
Thu 7 Dec	Current Issues 7 - Impact of shale gas and oil (Report 7 Due; Bonus Report
	Due)

# **Homework Reports:**

- Report 1 Industry Structure and Statistics (Due 31 August)
- Report 2 Reaction Path Synthesis: Solvay Process (Due 14 September)
- Report 2 Reaction 1 am Synthesis: Solvay 1 rocess (Dae 14 September)
  Report 3 Block Flow Diagram: Petroleum Refining (Due 28 September)
  Report 4 Process Supply Chain: Polyethylene Terephthalate (Due 12 October)

Report 5 - General Purpose Batch Processing: Fine Chemical Manufacture (Due 26 October)

Report 6 - Safety and Environmental Protection: Methyl Isocyanate (Due 9 November)

Report 7 - Sustainability: Carbon Management (Due 7 December)

Bonus Report: Process Narrative: Major Chemical Intermediate (Due 7 December)

# **Grading:**

20% Attendance and class participation 80% Reports (Report 7 counts double)

Bonus Report: Up to +10 percentage points

# **Academic Honesty:**

Students are individually responsible for each homework report. Cheating will not be tolerated. While discussions of homework among classmates are to be expected, students are responsible for submitting their own work. Copying the work of others, specifically including wholesale copying from electronic sources, is plagiarism and is considered a form of cheating.

#### **Accommodation:**

Purdue University strives to make learning experiences as assessable as possible. If you anticipate or experience physical or academic barriers based on disability, you are welcome to let the instructor know so that options may be discussed. You are also encouraged to contact the Disability Resource Center at <a href="mailto:drc@purdue.edu">drc@purdue.edu</a> or by phone at 765-494-1247.

In addition to the University policy, the Davidson School of Chemical Engineering has established procedures for students seeking accommodations. These can be found online at the ChE Undergrad Office website. Only those accommodation requests that conform to both University and ChE policy guidelines will be implemented.

#### **Protect Purdue:**

The Protect Purdue Plan, which includes the Protect Purdue Pledge, is a campus policy and as such all members of the Purdue community must comply with the required health and safety guidelines. Required behaviors in this class include: staying home and contacting the Protect Purdue Health Center if you feel ill or know you have been exposed to the virus, wearing a mask in classrooms and campus buildings at all times, disinfecting workspace prior to and after use, maintaining proper physical distancing, and maintaining robust personal hygiene. Measures will be taken to provide alternative remote instructional experiences if the course had an on-line delivery option or if on-line delivery becomes mandated during the course of the semester.

#### **References:**

Kirk-Othmer Encyclopedia of Chemical Technology (5<sup>th</sup> Ed and On-line, Wiley) Ullmann's Encyclopedia of Industrial Chemistry (5<sup>th</sup> Ed and On-line, Wiley) Shreve's Chemical Process Industries (5<sup>th</sup> Ed, McGraw-Hill Special Reprint Edition) Handbook of Chemical Technology and Pollution Control (Robert Myers, 3<sup>rd</sup> Ed, Elsevier) Handbook of Petroleum Refining Processes (Martin Hocking, 2<sup>nd</sup> Ed, McGraw Hill)

# **CHE 59700: Chemical Engineering Applications in Medical Devices**

- A. Instructors: William Clark, M.D. and Michelle Chutka
- **B.** Course Description. This course provides a unique perspective to the medical device field, with emphasis on the ways in which chemical engineering processes provide the foundation for many device-related therapies. The course involves the application of several fundamental chemical engineering principles, including those related to mass transfer, separations, and fluid flow, to devices used for extracorporeal therapies and other treatments. The first part of the course addresses the relevant physiology and pathophysiology serving as a foundation for subsequent clinical material. With the focus on extracorporeal devices, the interactions between blood and biomaterials in a general sense are also explored. The second part of the course assesses the extracorporeal treatment of kidney failure by dialysis, which is highlighted as the only long-term, device-based replacement therapy for terminal organ failure (end-stage renal disease). This analysis will not only consider the evolution of dialysis therapy from a technology perspective (with emphasis on fundamental chemical engineering principles) but also the forces that have shaped its development into a market generating annual revenue of nearly \$100 billion on a global basis. The third segment of the course addresses industry-focused concepts pertaining to medical device development, including the role of the chemical engineer in design verification and validation activities, process validations including IQ/OQ/PQ, risk analysis, lean manufacturing concepts, and project management in an increasingly complex regulatory environment. Providing a real-world perspective based on over 15 years of experience in the medical device field, Ms. Michelle Chutka (Director of Product Engineering, Cook Biotech, Inc; Continuing Lecturer, Davidson School of Chemical Engineering, Purdue University) will lead this third part of the course.
- C. Instructor Biographical Information: Dr. Clark is a nephrologist (kidney specialist) and chemical engineer by training. He received his M.D. degree along with specialty and sub-specialty training in internal medicine and nephrology, respectively, at Indiana University School of Medicine. In addition, he received both his B.S and M.S. degrees in chemical engineering from Purdue University, at which he is now Professor of Engineering Practice in the Davidson School of Chemical Engineering. Before joining the Purdue faculty, Dr. Clark worked in the medical device (dialysis) industry for more than 20 years in a variety of positions. During this time, he applied engineering principles to gain expertise in two broad areas, namely extracorporeal membrane structure/function and solute kinetics during dialysis. Dr. Clark continues to serve as a consultant in the dialysis industry.

Ms. Chutka is a chemical engineer by training with both B.S and M.S degrees from the University of Michigan. For the past 17 years, she has held roles of increasing responsibility at Cook Biotech, a medical device company based in West Lafayette, IN. In her current position as Director of Product Engineering, Ms. Chutka oversees the product engineering team, responsible for both upstream and discovery work, all aspects of product development through regulatory approval and commercialization, along with sustaining engineering for all aspects of the medical device's product lifecycle. Outside of medical device experience, Ms. Chutka has also worked in the pharmaceutical industry and abroad within the automotive industry.

**D. Prerequisites.** CHE 37700 (or equivalent) and BIOL 23000 (or BCHM 30700). These are not strict requirements - interested students should contact Dr. Clark with inquiries.

# E. Recommended (NOT REQUIRED) Texts.

- Guyton and Hall Textbook of Medical Physiology, Edited by John E. Hall, Elsevier, 2016, ISBN: 978-1-4557-7005-2
- Medical Device Development, Edited by Jonathan S. Kahan, Barnett International, 2009, ISBN: 1-882615-92-
- Biomaterials Science: An Introduction to Materials in Medicine, Edited by Buddy Ratner, Allan Hoffman, Frederick Schoen, Jack Lemons, Elsevier, 2012, ISBN: 978-0-12-374626-99

#### F. Course Learning Outcomes

Assess the mechanisms of blood-surface interactions defining the biocompatibility of an extracorporeal device

- Evaluate the influence of extracorporeal membrane structure and material on transport properties (diffusion, convection, and ultrafiltration) and the overall effect on device performance
- Based on a mass balance approach, analyze device-related and patient-related (physiologic) parameters required for kinetic modeling of different dialysis therapies
- Apply fundamental chemical engineering principles to provide a quantitative basis for treatments of specific clinical disorders, including end-stage renal disease (ESRD), acute kidney injury (AKI), sepsis, cardiac failure, and respiratory failure
- Characterize the major components of a medical device company and the manner in which these different functions interact during the pre-market and post-market phases of product development
- From the perspective of a chemical engineer working in the medical device field, understand how the principles of project management, verification/validation, process validation, risk analysis, and lean manufacturing pertain to product development and the regulatory approval process.

# G. Course Meeting Schedule

Lectures: Tues/Thurs 3:00-4:15 PM Homework 1: due February 6 Homework 2: due February 27 Homework 3: due April 3 Homework 4: due April 24

Presentation 1: March 9 (8-10 PM) Presentation 2: April 20 (8-10 PM)

Final Report due: May 3

Early in the semester, students will assemble into groups of 3 and choose a medical device-based clinical therapy to study. Each group will provide two progress updates (Presentations 1 and 2) during the course of the semester in lieu of formal examinations. A complete written summary of each group's assessment (Final Report) will be due at semester's end in lieu of a final examination.

#### **H.** Instructor Contact Information.

Professor William R. Clark – Email: clarkw@purdue.edu, Telephone: (765) 496-8647 (office); (317) 691-1438

(cell); office: FRNY 1055

Professor Michelle Chutka - Email: mchutka@purdue.edu

Office Hours: by appointment

**I. Assessment of Course Outcomes.** A weighted average grade will be calculated as follows.

Homework (4): 5% each = 20% total Presentations (2): 20% each = 40% total

Final report: 40%

### The grading scale will be as follows.

A: 100 - 85% of the weighted points

B: 84.9 - 75% of the weighted points

C: 74.9 - 65% of the weighted points

D: 64.9 - 55% of the weighted points

F: Less than 55% of the weighted points

Note that students with grades within 3 weighted percentage points of either the upper or lower bounds of a grade range listed above will receive a "plus" or "minus" mark, respectively, after his/her score (*e.g.*, scores between 75% and 78% of the total weighted points would earn an B—). Marks of an A— will not be given.

# Group projects

Student groups may assess a medical device-based therapy from a suggested list prepared by Professor Clark or choose one on their own. In either case, each group should plan to meet with Professor Clark before beginning work on the project to set expectations. The assessment will include the disease state(s) for which the technology is used, its historical development and evolution, the engineering principles underlying its use, the clinical challenges associated with the device, and potentially improved designs for the future. Requirements for the presentations during the semester and the final written summary will be provided early in the semester.

#### J. Class Schedule.

- January 10: Introduction
- January 12: Physiology overview (I)
- January 17: Physiology overview (I)
- January 19: Physiology overview (III)
- January 24: Interactions of blood with biomaterials (I)
- January 26: Interactions of blood with biomaterials (II)
- January 31: Kidney structure/function
- February 2: Normal kidney function
- February 7: Chronic kidney disease (CKD) and end-stage renal disease (ESRD)
- February 9: Uremic toxins: Chemical structure and clinical relevance
- February 14: Hemodialysis membrane properties
- February 16: Hemodialysis mass transfer
- February 21: Hemodialysis dose: Mass balance principles
- February 23: Extracorporeal therapy for AKI
- February 28: New device approaches for ESRD and AKI
- March 2: Extracorporeal therapies beyond renal failure
- March 7: Vascular access for dialysis
- March 9: Drug/device combinations
- March 9 (8-10 PM): Presentation #1
- March 14: Spring Break
- March 16: Spring Break
- March 21: Medical device regulation and clinical trials (I)
- March 23: Medical device regulation and clinical trials (II)
- March 28: Medical device market dynamics
- March 30: Medical device product development: Design verification/validation (I)
- April 4: Medical device product development: Design verification/validation (II)
- April 6: Medical device product development: Process Validation (I)
- April 11: Medical device product development: Process Validation (II)
- April 13: Applying risk analysis to device design (I)
- April 18: Lean manufacturing in the medical device industry, project management & regulatory strategy
- April 20: Case study
- April 20 (8-10 PM): Presentation #2
- April 25: No class
- April 27: No class

# CHE 59700-030 (3 credit-hours) Financial Analysis and Project Management Spring 2023

Class Location/ Format	FRNY 1043 – with WebEx link for guest lecturers
When	Monday, Wednesday, Friday
	11:30p – 1:00p
Duration	January 9, 2023 – March 4, 2023
Exam Format	Interim and Final Presentations (in-class)
	Final Paper

# **Primary Instructor**

#### Michelle Chutka

Email: <a href="mailto:mchutka@purdue.edu">mchutka@purdue.edu</a> Office Hours: By request

Michelle Chutka, M.S., is a graduate of the University of Michigan Chemical Engineering program (B.S. 2002, M.S, 2003). She has 17 years of experience in Medical Device industry, and is presently the Director of Product Engineering at Cook Biotech in West Lafayette, IN. She joined Purdue as a Continuing Lecturer in Fall 2019 and works closely with students pursuing the Professional Master's Program.

# **Featured Guest Lecturer**

# **Charlie Smith**

Email: <charlie4129@yahoo.com> Office Hours: 10:30-11:15am 1043 FRNY

Charlie Smith is a featured lecturer and former CEO of Countrymark. He has also served on the Board of the Indiana Chamber of Commerce, including the committees for Congressional Affairs and Energy, the Indiana University Kelly School of Business (Indianapolis) Board of Visitors, the Board of the Michigan Oil and Gas Association, and the Industry Advisory Council for Purdue University's School of Chemical Engineering. In 2015, the Purdue University Davidson School of Chemical Engineering honored Charlie as an Outstanding Chemical Engineer.

# **Featured Faculty**

Dr. William (Bill) Clark

Office: FRNY 2158 Email: <a href="mailto:clarkw@purdue.edu">clarkw@purdue.edu</a>

Dr. William Clark joined the Davidson School of Chemical Engineering in 2017 as a Visiting Professor. He received his B.S. and M.S. degrees in chemical engineering from Purdue and his medical degree from Indiana University, where he also received post-graduate training in internal medicine and nephrology (kidney disease). He held a variety

of positions at Baxter Healthcare and subsidiaries for 20 years, working exclusively in the dialysis field.

# **Course Description**

In both industry and academic settings, outcomes and goals are attained through project management. The goal of this course is to teach foundations of project management through a variety of case studies and course work, including financial analysis methods used to make investment decisions and discern opportunities for cash flow analysis. Businesses and other undertakings thrive through creating customer value. This course will challenge students to examine methods of creating customer value through assuming different roles within an organization.

At the beginning of the course, students will work both in teams and as individuals to analyze the financial reporting of a publicly traded entity. Students will be expected to provide one mid-point report as well as one final report regarding their recommendations for investments and management of that entity's portfolio.

# **Course Objectives**

Following the successful completion of this course, the student will achieve the following course objectives:

- 1. Understand the role of the engineer in creating value for an organization.
- 2. Understand and apply basic accounting principles to analyzing cash flows and balance sheets. Distinguish between managerial accounting and GAAP accounting principles.
- 3. Apply future and present valuation methods towards project selection.
- 4. Gain skills in proactive and reactive project selection using new analytical skills.
- 5. Grow engineering project management skills with focus on application tools.
- 6. Apply newfound analytical perspective towards an organization's financial health.

# Course Format

The format of this class will be a mix of in-person and synchronous lectures. Many guest lecturers will provide content that is available only through online meetings, and these lectures will be performed exclusively over an online platform with an asynchronous option if the guest lecturer consents to information sharing. We will have opportunities to meet and discuss content in-person as well.

The guest lecturers will discuss a wide range of issues, including investments and the stock market, corporate taxes, the start-up process, entrepreneurship, mergers and acquisitions, private equity, hedge funds, venture capital, strategic risk, and assessment of funding for R&D investments. Several companies will be specifically highlighted during

these guest lectures, including representatives from Consumer Goods, Pharma/Med Device, Energy and Petroleum industries.

# Prerequisites

Ability to use EXCEL or hand-calculate simple problems. Some background in general accounting principles may be helpful but is not required.

# Learning Outcomes

#### Students will learn to:

- Interpret and understand financial earnings statements
- Think of projects in an expansive way where projects can be new business lines, improvements in existing businesses, start-ups, partnerships and capital expenditures of any size
- Do project analysis including economic evaluations
- Balance quantitative analysis with business judgment
- Distinguish between project management practices that have a good chance of success from those that are less likely to succeed
- Learn how to assess and manage risks

# Optional Textbook

- Stermole et al. Economic Evaluation & Investment Decisions Methods Edition 16
- \*\*This particular edition will be reference in class, but Edition 16 is not required. Much of the content is available in previous editions if easier to obtain.

#### **Optional Texts**

- "Finance for Executives," Hawawini and Viallet 5<sup>th</sup> edition Selected Chapters
- "Sources of Value, A Practical Guide to the Science and Art of Valuation,"
   Woolley, Cambridge, 2009 selected chapters from this book may be used, and will be uploaded to Brightspace
- "Project Management for the Unofficial Project Manager," 2015, Franklin Covey
   Co. Selected excerpts will be discussed in class.

# **Policies**

#### **General Course Policies**

We expect the highest standards of professionalism and ethics in this course. Each student is expected to come to class on time and participate in lectures and content. Each student is also expected to follow Purdue's codes of student conduct (<a href="http://www.purdue.edu/studentregulations/student\_conduct/regulations.html">http://www.purdue.edu/studentregulations/student\_conduct/regulations.html</a>) and behave in a professional manner. The rights of students in violation of the code of conduct are outlined. Each student is expected to exhibit consideration and respect towards the ChE 59700-030 Spring 2023

other students, the graders, the teaching assistants (TAs), and the faculty members. Each student is expected to exhibit a positive attitude. Expectations for each student include (but are not limited to):

- Attending all class sessions.
- Coming to on time and prepared by reading assigned material beforehand.
- Participating in classes and online lectures through posing questions and engaging in course material.
- Maintaining the highest standards of academic honesty and integrity.
- Being knowledgeable about the policies and information described in the syllabus.

# Grading

Course participation is a critical portion of this course, even classes held online or asynchronously!

Course participation grades will be assessed through confirmation that you've engaged the recorded/asynchronous or synchronous lectures. Lectures given in an asynchronous format for those unable to attend in-person are to be reviewed with the expectation that the student engages the content and returns with questions for the lecturer.

The lecturers may use discussion forums on Brightspace to provide tools and opportunities for enrichment. Discussion on these forums outside of coursework is encouraged and will count favorably towards class participation grades.

Grading rubric is illustrated below:

Class Activity	Approximate Total Grade Weight
Class participation, including: - Attendance and participation in lectures - Completing assigned reading - Discussion/engagement on Brightspace	10%
Homework	20%
Mid-Point Presentation 1	20%
Final Presentation 2	20%
Final Paper	30%

Letter Grade Range	Grade Range
A range	100% - 90.0%
A- range/B+ range	89.9% - 85.1%
В	85.0% - 75.0%
С	74.9% - 65.0%
D	64.9% - 55.0%
F	<55.0%

<sup>\*</sup>Unless otherwise specified, a letter grade may be assigned with a + or – contingent upon class participation and engagement, among other factors.

If an assignment or homework was too difficult (as judged by the faculty instructors) the final grade may be scaled to a higher value. Grades will never be scaled downward. As a rule, scaling will not be applied. There is no preset distribution of final grades. The grading will reflect demonstrated student capability relative to an absolute performance standard that is expected of all Purdue chemical engineering students, rather than a scale that compares students to a mean performance metric on any evaluation vehicle. In practice, this means the entire class could receive A marks.

For the presentations, students will collaboratively analyze a chosen publicly traded entity. While each student is free to decide what aspects of a company will be assessed, basic expectations include a review of recent financial statements and a critical analysis of the company's strategy over time. Each student's work will be summarized in a series of presentations. More details about the expectations for the presentations will be provided during the first week of class.

The final paper will be written and submitted <u>individually</u> <u>by each team member</u> and include a summary of the team's findings and progress throughout the semester. This paper will be due prior to the end of the grading period for the Spring 2022 semester.

#### **Instructor's Commitment**

As your instructor, I hold myself to the highest standards and expectations to provide a model for student behavior. These commitments include, but are not limited to:

- exhibiting punctuality and preparedness for lectures, both in content and knowledge.
- providing a safe and open forum for learning. No student should feel ashamed or embarrassed to ask a question, for any reason.
- providing timely responses to email or in-person inquiries. If class time is not the best forum to answer these questions, a suitable time outside of class will be chosen.
- grading with objectivity and consistency based on pre-determined guidelines.

### **Instructor Questions & Office Hours.**

The best way to reach Michelle is by email <a href="mailto:mchutka@purdue.edu">mchutka@purdue.edu</a>. I will arrange a Teams discussion if an email discussion is not convenient or effective. Expect a response within 24 to 48 hours on business days. Guest lecturers will also be available for subsequent consult.

### **Academic Dishonesty**

Academic dishonesty <u>will not be tolerated in any form in this course.</u> Specifically, Purdue prohibits "dishonesty in connection with any University activity. Cheating, plagiarism, or knowingly furnishing false information to the University are examples of dishonesty." [Section B-2-a, Code of Student Conduct] Furthermore, the University Senate has stipulated that "the commitment of acts of cheating, lying, and deceit in any of their diverse forms (such as the use of substitutes for taking examinations, the use of illegal cribs, plagiarism, and copying during examinations) is dishonest and must not be tolerated. Moreover, knowingly to aid and abet, directly or indirectly, other parties in committing dishonest acts is in itself dishonest." [University Senate Document 72-18, December 15,

1972] All incidents of academic dishonesty will be reported to the Dean of Students. <u>Such</u> incidents include:

- (i) <u>possessing or accessing, in hardcopy or electronic form, the solution manual</u> to the course text, or to the exams;
- (ii) claiming credit for work that is not your own original work;
- (iii) enabling other students to create work that is not their original work.

The punishment for the first offense is a grade of zero for the entire work (exam or homework), and the punishment for a second offense is an F mark for the class.

Refer to Purdue's student guide for academic integrity: https://www.purdue.edu/odos/academic-integrity/

# **Use of Copyrighted Materials**

Students are expected, within the context of the Regulations Governing Student Conduct and other applicable University policies, to act responsibly and ethically by applying the appropriate exception under the Copyright Act to the use of copyrighted works in their activities and studies. The University does not assume legal responsibility for violations of copyright law by students who are not employees of the University.

A Copyrightable Work created by any person subject to this policy primarily to express and preserve scholarship as evidence of academic advancement or academic accomplishment. Such works may include, but are not limited to, scholarly publications, journal articles, research bulletins, monographs, books, plays, poems, musical compositions and other works of artistic imagination, and works of students created in the course of their education, such as exams, projects, theses or dissertations, papers and articles.

You may want to refer students to the University Regulations on policies: <a href="http://www.purdue.edu/policies/academic-research-affairs/ia3.html">http://www.purdue.edu/policies/academic-research-affairs/ia3.html</a>

#### Attendance

Students are expected to be present for every meeting of the classes in which they are enrolled. Only the instructor can excuse a student from a course requirement or responsibility. When conflicts or absences can be anticipated, such as for many University sponsored activities, an interview or religious observations, the student should inform the instructor of the situation as far in advance as possible. For unanticipated or emergency absences when advance notification to an instructor is not possible, the student should contact the instructor as soon as possible by email. When the student is unable to make direct contact with the instructor and is unable to leave word with the instructor's department because of circumstances beyond the student's control, and in cases of bereavement, the student or the student's representative should contact the Office of the Dean of Students.

The link to the complete policy and implications can be found at: <a href="http://www.purdue.edu/studentregulations/regulations">http://www.purdue.edu/studentregulations/regulations</a> procedures/classes.html

#### **Missed or Late Work**

All assignments must be completed and submitted on time. As a rule, late submissions will not receive credit. Assignments will be submitted through Brightspace by the time and date indicated on the assignment. If an extreme circumstance arises, contact the Professor.

# **Grief Absence Policy for Students**

Purdue University recognizes that a time of bereavement is very difficult for a student. The University therefore provides the following rights to students facing the loss of a family member through the Grief Absence Policy for Students (GAPS). GAPS Policy: Students will be excused for funeral leave and given the opportunity to earn equivalent credit and to demonstrate evidence of meeting the learning outcomes for missed assignments or assessments in the event of the death of a member of the student's family.

See the University's website for additional information: <a href="http://www.purdue.edu/studentregulations/regulations">http://www.purdue.edu/studentregulations/regulations</a> procedures/classes.html

# **Violent Behavior Policy**

Purdue University is committed to providing a safe and secure campus environment for members of the university community. Purdue strives to create an educational environment for students and a work environment for employees that promote educational and career goals. Violent Behavior impedes such goals. Therefore, Violent Behavior is prohibited in or on any University Facility or while participating in any university activity.

See the University's website for additional information: http://www.purdue.edu/policies/facilities-safety/iva3.html

# **Emergencies**

In the event of a major campus emergency, course requirements, deadlines and grading percentages are subject to changes that may be necessitated by a revised semester calendar or other circumstances beyond the instructor's control. Relevant changes to this course will be posted onto the course website or can be obtained by contacting the instructors via email or phone. You are expected to read your @purdue.edu email on a frequent basis.

See the University's website for additional information: <a href="https://www.purdue.edu/ehps/emergency">https://www.purdue.edu/ehps/emergency</a> preparedness/

#### Students with Disabilities

Any academic accommodation must be arranged for <u>by the student</u> through Purdue's Disability Resource Center. Instructors cannot make academic accommodations without a DRC accommodation letter. Below is Purdue's policy statement for supporting students with disabilities.

Purdue University is committed to maintaining an inclusive community that recognizes and values the inherent worth and dignity of every person; fosters tolerance, sensitivity, understanding and mutual respect among its members; and encourages each individual

to strive to reach his or her own potential. In pursuit of its goal of academic excellence, Purdue University seeks to develop and nurture its diversity. The University believes that diversity among its many members strengthens the institution, stimulates creativity, promotes the exchange of ideas and enriches campus life.

Purdue University views, evaluates and treats all persons in any university-related activity or circumstance in which they may be involved solely as individuals on the basis of their own personal abilities, qualifications and other relevant characteristics.

Purdue University does not condone and will not tolerate Discrimination against any individual on the basis of race, religion, color, sex, age, national origin or ancestry, genetic information, disability, status as a veteran, marital status, parental status, sexual orientation, gender identity or gender expression. Purdue University promulgates policies and programs to ensure that all persons have equal access to its employment opportunities and educational programs, services and activities. The principal objective of this policy is to provide fair and consistent treatment for all students and employees of the University. Purdue is committed to increasing the recruitment, selection and promotion of faculty and staff at the University who are racial or ethnic minorities, women, persons with disabilities and veterans. The University also is committed to policies and programs that increase the diversity of the student body.

Here are some links that may be relevant:

http://www.purdue.edu/policies/ethics/iiic2.html

http://www.purdue.edu/studentregulations/equal opportunity/studentgrievance.html

https://www.purdue.edu/studentsuccess/specialized/drc/faculty/index.html

#### Nondiscrimination

Purdue University is committed to maintaining a community which recognizes and values the inherent worth and dignity of every person; fosters tolerance, sensitivity, understanding, and mutual respect among its members; and encourages each individual to strive to reach his or her own potential. In pursuit of its goal of academic excellence, the University seeks to develop and nurture diversity. The University believes that diversity among its many members strengthens the institution, stimulates creativity, promotes the exchange of ideas, and enriches campus life.

Purdue University prohibits discrimination against any member of the University community on the basis of race, religion, color, sex, age, national origin or ancestry, genetic information, marital status, parental status, sexual orientation, gender identity and expression, disability, or status as a veteran. The University will conduct its programs, services and activities consistent with applicable federal, state and local laws, regulations and orders and in conformance with the procedures and limitations as set forth in Executive Memorandum No. D-1, which provides specific contractual rights and remedies. Any student who believes they have been discriminated against may visit <a href="https://www.purdue.edu/report-hate">www.purdue.edu/report-hate</a> to submit a complaint to the Office of Institutional Equity. Information may be reported anonymously.

You may want to refer students to Purdue's nondiscrimination statement: <a href="http://www.purdue.edu/purdue/ea">http://www.purdue.edu/purdue/ea</a> eou statement.html



#### **EMERGENCY PREPAREDNESS SYLLABUS ATTACHMENT**

EMERGENCY NOTIFICATION PROCEDURES are based on a simple concept – if you hear a fire alarm inside, proceed outside. If you hear a siren outside, proceed inside.

- **Indoor Fire Alarms** mean to stop class or research and <u>immediately</u> **evacuate** the building.
- Proceed to your Emergency Assembly Area away from building doors. Remain outside until police, fire, or other emergency response personnel provide additional guidance or tell you it is safe to leave.
- All Hazards Outdoor Emergency Warning Sirens mean to <u>immediately</u> seek shelter (Shelter in Place) in a safe location within the closest building.
  - "Shelter in place" means seeking immediate shelter inside a building or University residence. This course of action may need to be taken during a tornado, a civil disturbance including a shooting or release of hazardous materials in the outside air. Once safely inside, find out more details about the emergency\*. Remain in place until police, fire, or other emergency response personnel provide additional guidance or tell you it is safe to leave.

\*In both cases, you should seek additional clarifying information by all means possible...Purdue Emergency Status page, text message, Twitter, Desktop Alert, Albertus Beacon, digital signs, email alert, TV, radio, etc....review the Purdue Emergency Warning Notification System multi-communication layers at <a href="http://www.purdue.edu/ehps/emergency">http://www.purdue.edu/ehps/emergency</a> preparedness/warning-system.html

#### **EMERGENCY RESPONSE PROCEDURES:**

- Review the Emergency Procedures Guidelines
   https://www.purdue.edu/emergency\_preparedness/flipchart/index.html
- Review the **Building Emergency Plan** (available on the Emergency Preparedness website or from the building deputy) for:
  - o evacuation routes, exit points, and emergency assembly area
  - when and how to evacuate the building.
  - shelter in place procedures and locations
  - o additional building specific procedures and requirements.

#### **EMERGENCY PREPAREDNESS AWARENESS VIDEOS**

• "Shots Fired on Campus: When Lightning Strikes," is a 20-minute active shooter awareness video that illustrates what to look for and how to prepare and react to this type of incident. See: <a href="http://www.purdue.edu/securePurdue/news/2010/emergency-preparedness-shots-fired-on-campus-video.cfm">http://www.purdue.edu/securePurdue/news/2010/emergency-preparedness-shots-fired-on-campus-video.cfm</a> (Link is also located on the EP website)

#### **MORE INFORMATION**

Reference the Emergency Preparedness web site for additional information: https://www.purdue.edu/ehps/emergency\_preparedness/

# **CHE597 Computational Optimization, Spring 2024**

**Instructor:** Can Li **Email:** canli@purdue.edu

# **Course Description:**

This is a graduate-level introductory course to mathematical optimization. We will cover the theory and algorithms of linear programming, mixed-integer linear/nonlinear programming, conic programming, global optimization of nonconvex problems, and decomposition algorithms for mixed-integer programs. Special focus will be given to using the APIs of modern computational software including CPLEX, Gurobi, Mosek, Pytorch with implementations in Python. We will motivate the algorithms using modern applications in chemical engineering, transportation, energy systems, machine learning, and control.

The course lectures will be 30% proofs, 50% algorithms and computation, and 20% modeling and applications in engineering. The homework will keep a similar portion. However, we will not have proofs in the exams since this is a class targeted at engineering students.

#### <u>Topics Covered (tentative)</u>

# **Optimization basics**

- Convex sets, functions
- Unconstrained optimization, gradient descent, Newton's method
- Simple applications of optimization models
- Modeling using pyomo

#### Linear and conic programming

- Applications
- Basics of polyhedral theory, LP duality
- Second-order cone programming (SOCP)
- Semidefinite programming (SDP), Goemans-Williamson

### **Nonlinear programming**

- Applications
- Optimality conditions
- Barrier algorithm, interior point algorithm

# (Mixed)-integer linear programming

- Modeling of discrete and continuous decisions
- Propositional logic, modeling of disjunctions
- Applications
- Branch and bound
- Cutting planes
- Disjunctive programming

# **Global optimization of nonconvex problems**

- Applications
- Convex relaxations, McCormick Inequality
- Spatial branch and bound
- Mixed-integer nonlinear programming

# **Decomposition algorithms**

- Benders decomposition, stochastic programming
- Dantzig Wolfe decomposition, column generation, vehicle routing problems
- Lagrangian decomposition
- ADMM

# **Advanced topics on computation**

- Numerical linear algebra
- Advanced solver callbacks
- Parallel computing
- GPU computing

#### **Recommended Textbooks:**

This class will not exactly follow any textbook. But we may cover some of the content in the following textbooks.

- 1. Grossmann, I. E. (2021). Advanced optimization for process systems engineering. Cambridge University Press.
- 2. Wolsey, L. A. (2020). Integer programming. John Wiley & Sons.
- 3. Bertsimas, D., & Tsitsiklis, J. N. (1997). Introduction to linear optimization (Vol. 6, pp. 479-530). Belmont, MA: Athena scientific.
- 4. Ben-Tal, A., & Nemirovski, A. (2001). Lectures on modern convex optimization: analysis, algorithms, and engineering applications. Society for industrial and applied mathematics.
- 5. Conforti, M., Cornuéjols, G., Zambelli, G., Conforti, M., Cornuéjols, G., & Zambelli, G. (2014). Integer programming models (pp. 45-84). Springer International Publishing.

#### Software

We will use the following software

- <u>Pyomo</u> is a collection of Python software packages for formulating optimization models. Tutorial: <u>ND Pyomo</u>
   Cookbook
- <u>Gurobi</u> and <u>Cplex</u> are both high-performance mathematical programming solver for linear programming, mixed integer programming, and quadratic programming.
- <u>Mosek</u> is a software package for the solution of linear, mixed-integer linear, quadratic, mixed-integer quadratic, quadratically constraint, conic and convex nonlinear mathematical optimization problems.

### **Prerequisite**

Some familiarity with linear algebra, calculus, and programming in python is required.

• YouTube videos review of linear algebra and calculus by 3Blue1Brown

- <u>Linear algebra review</u> videos by Zico Kolter
- General mathematical review: Appendix A of Boyd and Vandenberghe (2004)

### **Related courses**

- <u>Convex optimization</u> by Ryan Tibshirani
- <u>Convex analysis</u> by Dimitri Bertsekas
- <u>Linear programming</u> by Santanu Dey
- <u>Integer programming</u> by Ted Ralphs
- <u>Linear and convex optimization classes</u> by Arkadi Nemirovski

Last updated: October 12, 2023

Any updates to this may be at this url

https://canli1.github.io/courses

# Colloidal and Interfacial Phenomena

**Instructor:** Professor You-Yeon Won; Room 2031 FRNY

Tel: 4-4077; email: yywon@purdue.edu

Office hours: T 7:30 – 8:20 PM (virtual, subject to occasional changes,

https://purdue.webex.com/purdue/j.php?MTID=mc678d1347b8c42d35b623626e8ac195f)

**Classes:** M, W, F 11:30 AM – 12:20 PM, HAMP 2118

**Teaching Assistants:** No graduate TA has been assigned for this course this year.

**Prerequisites:** Undergraduate physical chemistry

#### Text:

D. F. Evans, and H. Wennerström, "The Colloidal Domain: Where Physics, Chemistry, Biology, and Technology Meet", 2<sup>nd</sup> ed., Wiley-VCH, 1999 (on reserve in Engineering Library).

#### **Supplemental Text:**

- R. J. Stokes, and D. F. Evans, "Fundamentals of Interfacial Engineering", Wiley-VCH, 1996 (on reserve in Engineering Library).
- P. C. Hiemenz, and R. Rajagopalan, "Principles of Colloid and Surface Chemistry", 3<sup>rd</sup> ed., CRC Press, 1997 (on reserve in Engineering Library).

#### **Additional References:**

- J. Israelachvili, "Intermolecular & Surface Forces", 3rd ed., Academic Press, 2011.
- K. A. Dill, and S. Bromberg, "Molecular Driving Forces: Statistical Thermodynamics in Chemistry and Biology", 2<sup>nd</sup> ed., Garland Science, 2010.
- V. A. Parsegian, "Van Der Waals Forces: A Handbook for Biologists, Chemists, Engineers, and Physicists", Cambridge University Press, 2006.
- M. Rubinstein, and R. H. Colby, "Polymer Physics", Oxford University Press, 2003.
- T. A. Witten, "Structured Fluids: Polymers, Colloids, Surfactants", Oxford University Press, 2004.
- P.-G. de Gennes, F. Brochard-Wyart, and D. Quere, "Capillary and Wetting Phenomena: Drops, Bubbles, Pearls, Waves", Springer, 2004.
- B. W. Ninham, and P. Lo Nostro, "Molecular Forces and Self-Assembly: In Colloids, Nano Sciences and Biology", Cambridge University Press, 2010.
- H. Bechhold, "Colloids in Biology and Medicine", D. Van Nostrand Company, 1919 (translation from the 2<sup>nd</sup> German edition).
- W. Norde, "Colloids and Interfaces in Life Sciences", Marcel Dekker, 2003.
- H. C. Berg, "Random Walks in Biology", Princeton University Press, 1993.

- W. M. Saltzman, "Drug Delivery: Engineering Principles for Drug Delivery", Oxford University Press, 2001.
- B. J. Berne, and R. Pecora, "Dynamic Light Scattering: With Applications to Chemistry, Biology, and Physics", Dover Publications, 2000.
- P. C. Hiemenz, and T. P. Lodge, "Polymer Chemistry", 2nd ed., CRC Press, 2007.

# **Course Objectives:**

- 1. Develop a broad understanding of core principles/concepts, and experimental techniques, relevant to the studies of colloidal and interfacial phenomena (see the course outline below for specific topics that will be covered).
- 2. Learn about current topics in colloid and interface science (relevant reading materials from contemporary research literature will be handed out throughout the semester).

Tentative Course Outline: (subject to changes)

<u>Tentative Course Outline:</u> (subject to changes)			
Weeks of	Topics		
1/10	0.	O. Introduction (definition, examples, history)	
	1.	Forces between molecules & between particles	
1/10, 1/17, 1/23, 1/31		1.1 van der Waals (vdW) forces	
(No class on 1/17: Martin		1.1.1 vdW forces between molecules in vacuum	
Luther King Jr. Day)		(Keesom (orientation)/Debye	
		(induction)/London (dispersion) interactions)	
		1.1.2 vdW forces between particles in vacuum	
		1.1.3 vdW forces between particles in solvent	
1/31, 2/7		1.2 Forces between charged particles in electrolyte	
		solutions	
		1.2.1 Electrostatic force	
		1.2.2 Osmotic force	
		1.2.3 DLVO theory	
		1.2.4 Surface chemistry & chemical specificity	
2/14, 2/21		1.3 Steric polymeric force	
2/21, 2/28		1.4 Hydration force	
		1.4.1 Hydrophobic hydration of small non-polar	
		molecules	
		1.4.2 Hydrophobic hydration of larger particles	
2/28, 3/7		1.5 Other forces	
		1.5.1 Solvent packing force	
		1.5.2 Undulation force	
		1.5.3 Depletion force	
	2.	Phenomena involving collections of molecules &	
		particles	
3/7, 3/21		2.1 Coagulation & ordering of particles	
(Midterm exam on 3/10)		2.1.1 Kinetics of coagulation of particles	
(No classes on 3/14, 3/16,		2.1.2 Structures of aggregates	
3/18: Spring Vacation)		2.1.3 Concentration-dependent phase behaviors of colloids	
3/28, 4/4, 4/11	2.2 Capillarity, wetting, & insoluble monolayers		

		2.2.1 Surface tension	
		2.2.2 Cohesion, adhesion, spreading	
		2.2.3 Capillarity	
		2.2.4 Insoluble monolayers	
		2.2.5 Amphiphilic assemblies	
	3.	Dynamics of particles & molecules in colloidal systems	
4/18		3.1 Microscopic theory	
., 10		3.1.1 Mean square displacement	
		3.1.2 Gaussian distribution	
4/18		3.2 Macroscopic theory	
		3.2.1 Fick's law equations	
		3.2.2 Diffusion to a spherical absorber	
4/18		3.3 Diffusion coefficient from first principles: Stokes-	
		Einstein equation	
		3.3.1 Diffusion as thermal drift	
		3.3.2 Viscous drag coefficient	
4/25		3.4 Sedimentation	
		3.4.1 Sedimentation velocity	
		3.4.2 Sedimentation equilibrium	
	4.	Measurements of structures & dynamics of colloids	
4/25		4.1 Light scattering	
		4.1.1 Static light scattering (if time allows)	
		4.1.2 Dynamic light scattering	
4/25		4.2 Rheology of suspensions and gels/networks (if time	
(Final exam on 4/29)		allows)	

#### **Grades:**

The course grade will be based on homework (20%), one midterm (30%), one final (40%), and class participation (10%). Attendance is required. For every unexcused absence, your final grade will be reduced by one point (out of 100). This course will use a +/- grading system.

#### Home work:

There will be 4–5 homework sets, due 2–3 weeks after assigned. *On each homework assignment, students are required to do all problems, but only part of the assigned problems will be graded*. Solutions to some problems will be handed out before examination. Some exam questions will be derived from homework problems. General discussion between students is encouraged, but homework should be done independently, unless directed otherwise. Copying will result in heavy penalty for all involved. All homework must be submitted via email to <a href="mailto:yywon@purdue.edu">yywon@purdue.edu</a> (as an attachment in PDF format) before class on the due date. Please use the following filename format: e.g., "CHE 668 Homework 1 YOUR LAST NAME.pdf".

#### Exams:

The midterm exam will take place on the evening of Thursday 3/10 (time & location: TBD). The final exam will also take place during the class on Friday 4/29. All exams will be closed

book and closed notes, but students will be allowed to have one double-sided  $3" \times 5"$  note card with information on it.

### **Unethical Conduct:**

Any activity in which a student seeks credit for work performed in the unjust manner (or helps another student to do so) constitutes cheating. This includes falsifying class attendance records, and using aides during exams. Students caught cheating will be prosecuted to the maximum extent possible under Purdue University guidelines. Punitive actions will include at minimum reduction of course grade but may include expulsion from the University.

#### **Communication Protocols:**

Please use the professor's office hours for additional help or for any questions or requests regarding the course. Please use email or phone only in case of personal issues that need to be urgently addressed. Emails that do not follow this protocol will be disregarded without reply. Also, emails that ask questions that are clearly and directly answered by the information in the syllabus will be disregarded without reply.

### **Campus Emergency:**

In the event of a major campus emergency (e.g., a pandemic), course requirements, deadlines and grading percentages are subject to changes that may be necessitated by a revised semester calendar or other circumstances. During such a disruption, information about changes in this course will be communicated by email.