CHE 525-Introduction to Biochemical Engineering

Instructor: Dr. Xiaoping Bao
Office: FRNY 1158
Office Phone: 496-3094
Email: bao61@purdue.edu

Course Meeting Time: 10:30-11:45 AM TR

Place: LAMB 108

Office Hours: virtual meetings by appointment.

Summary: Biochemical engineering is the field of study concerned with production or remediation of compounds using biological molecules and organisms. The purification of biomolecules is also an important area for biochemical engineers. This course will present a quantitative and mechanistic understanding of biological processes based on the core areas of chemical engineering; thermodynamics, kinetics, and transport phenomena. Topics that will be covered are enzyme kinetics coupled with mass transfer, modeling of microbial growth and mass balances, bioreactor design and operation, genetic and metabolic engineering, plant and animal cell culture and purification of bioproducts.

Text: Bioprocess Engineering, Basic Concepts *Third edition* (2017) M. Shuler, F. Kargi and M. DeLisa

Supplemental notes and articles will be posted on Brightspace or handed out during class.

Requirements: Assigned readings from the text and handouts are required. Problem sets will be assigned and are due one-week later at the beginning of class. No late homework will be accepted unless arranged with instructor prior to due date. An individual literature review project will be assigned on a topic of your choosing and will be due on the second day of the finals period.

Examinations: There will be two in class exams and no final exam. Occasionally students will have to miss an intra-semester exam for personal or uncontrollable reasons. However, if an exam needs to be missed, **NO make-up exams** allowed during the regular semester. **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 Bao. In this case, a **Final Exam** will be scheduled as a make-up exam.

Grading:
Exams (2): 60%
Homework (~9): 20%
Final Project: 20%

CHE 525 Syllabus

Week	T	R
01/19/2021	Introduction	Metabolism overview
1/26	Amino acids / Proteins	Enzymes
2/2	Enzyme Kinetics	
2/9	Biocatalysis	Immobilized Enzymes
2/16	Microbial Growth	
2/23	Batch reactors	Fed-batch
3/2	Chemostat Modeling	
3/9	Exam I	
3/16	Bioreactor Selection	Reading Day
3/23	Gas-Liquid Mass Transfer	Scale-Up
3/23	Instrumentation and Control	Solid State Fermentation
3/30	Sterilization	Bioseparations
4/6	Physical methods	
4/13	Reading Day	Chromatographic Separations
4/20	Animal Cell Culture	Exam II
4/27	Protein Engineering	Biotechnology Ethics
5/4	Final Week (Final Project Due)	

Literature Review Paper due: 5PM in my office on Tuesday of Finals Week

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.

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). 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.

Instructors' Commitment: 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 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.

Consulting with the Faculty Members: We encourage you to discuss academic or personal questions with us during class breaks, appointments or via email or Hotseat. These discussions need not be limited to ChE 525 content.

Statement of Academic Integrity

The commitment of acts of cheating, lying, and deceit in any of their diverse forms (such as the use of substitutes for taking examinations, use of illegal cribs, plagiarism and copying during homework, projects, or examinations is dishonest and will not be tolerated.

Definition of Academic Dishonesty

Purdue University prohibits dishonesty in connection with any University activity. Cheating, plagiarism or knowingly furnishing false information to the University are all examples of dishonesty. Knowingly aided or abetting cheating is also a dishonest act.

Students caught cheating will receive a zero for the assignment or exam for the first offense. Those caught a second time will automatically receive a failing grade for the course. Individual cases may be referred to the Dean of Students office for review and record keeping.

EMERGENCY PREPAREDNESS

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 immediately **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 immediately 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 Home page, email alert, TV, radio, etc…review the Purdue Emergency Warning Notification System multi-communication layers at http://www.purdue.edu/ehps/emergency_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 from the building deputy) for: ○ evacuation routes, exit points, and emergency assembly area
    - when and how to evacuate the building.
    - shelter in place procedures and locations
    - 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: http://www.purdue.edu/securePurdue/news/2010/emergency-preparedness-shots-fired-on-campus-video.cfm (Link is also located on the EP website)

MORE INFORMATION

Reference the Emergency Preparedness web site for additional information: http://www.purdue.edu/emergency_preparedness

COVID19-Related Important Notes

A. **Follow the Protect Purdue policy and measurements** (https://protect.purdue.edu/updates/)

B. **Academic Guidance in the Event a Student is Quarantined/Isolated**. If you become quarantined or isolated at any point in time during the semester, in addition to support from the Protect Purdue Health Center, you will also have access to an Academic Case Manager who can provide you academic support during this time. Your Academic Case Manager can be reached at acmq@purdue.edu and will provide you with general guidelines/resources around communicating with your instructors, be available for academic support, and offer suggestions for how to be successful when learning remotely. Importantly, if you find yourself too sick to progress in the course, notify your academic case manager and notify me via email or Brightspace. We will make arrangements based on your particular situation. The Office of the Dean of Students (odos@purdue.edu) is also available to support you should this situation occur.

C. **Attendance Policy during COVID-19**. Students should stay home and contact the Protect Purdue Health Center (496-INFO) if they feel ill, have any symptoms associated with COVID-19, or suspect they have been exposed to the virus. In the current context of COVID-19, in-person attendance will not be a factor in the final grades, but the student still needs to inform the instructor of any conflict that can be anticipated and will affect the submission of an assignment or the ability to take an exam. Only the instructor can excuse a student from a course requirement or responsibility. When conflicts can be anticipated, such as for many University-sponsored activities and religious observations, the student should inform the instructor of the situation as far in advance as possible. For unanticipated or emergency conflict, when advance notification to an instructor is not possible, the student should contact the instructor as soon as possible by email, through Brightspace, or by phone. 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, quarantine, or isolation, the student or the student's representative should contact the Office of the Dean of Students via email or phone at 765-494-1747. Our course Brightspace includes a link on Attendance and Grief Absence policies under the University Policies menu.

D. **Classroom Guidance Regarding Protect Purdue**.

The Protect Purdue Plan, which includes the Protect Purdue Pledge, is 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 (496-INFO) if you feel ill or know you have been exposed to the virus, properly wearing a mask in classrooms and campus building, at all times (e.g., mask covers nose and mouth, no eating/drinking in the classroom), disinfecting desk/workspace prior to and after use, maintaining appropriate social distancing with peers and instructors (including when entering/exiting classrooms), refraining from moving furniture, avoiding shared use of personal items, maintaining robust hygiene (e.g., handwashing, disposal of tissues) prior to, during and after class, and following all safety directions from the instructor.

Students who are not engaging in these behaviors (e.g., wearing a mask) will be offered the opportunity to comply. If non-compliance continues, possible results include instructors asking the student to leave class and instructors dismissing the whole class. Students who do not comply with the required health behaviors are violating the University Code of Conduct and will be reported to the Dean of Students Office with sanctions ranging from educational requirements to dismissal from the university.

Any student who has substantial reason to believe that another person in a campus room (e.g., classroom) is threatening the safety of others by not complying (e.g., not wearing a mask) may leave the room without consequence. The student is encouraged to report the behavior to and discuss next steps with their instructor. Students also have the option of reporting the behavior to the Office of the Student Rights and Responsibilities. See also Purdue University Bill of Student Rights.

Related Considerations:

1. *A listing of recommended safe practices for the specific class or laboratory setting (other PPE or safety behavior) can be found at the links below.*
    - Overarching SOP for Classrooms, Instructional Laboratories, and Experiential Courses
2. *References Supporting Protect Purdue Compliance:*
    - Office of the Dean of Students Protect Purdue Compliance Plan: Ask, Offer, Leave, Report
    - Office of the Dean of Students Managing Classroom Behavior and Expectations

E. Mental Health Statement.

If you find yourself beginning to feel some stress, anxiety and/or feeling slightly overwhelmed, try WellTrack. 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 Office of the Dean of Students. 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 Purdue Wellness Coach at RecWell. 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 evans240@purdue.edu.

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 Counseling and Psychological Services (CAPS) at 765-494-6995 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.

CHE 540: Transport Phenomena

Instructors:	Prof. Vivek Narsimhan Room FRNY 1029B Phone: 765-494-4281 Email: vnarsim@purdue.edu
TA	Isaac Wheeler Room FRNY 2121 Email: iwheeler@purdue.edu
Lectures:	Tues, Thurs 9:00 – 10:15 AM FRNY B124
Office Hours:	Prof. Narsimhan: Thurs 2:00 – 3:00 PM, FRNY 3062B Isaac: Fri 2:00 – 3:00 PM, FRNY 3062B
Recitation (optional)	Isaac: a few times this semester (Friday 3:00-4:00 PM,)

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

- Primary textbook 1: *Analysis of Transport Phenomena*, 2nd Ed, by William M. Deen, Chapters 1-12
- Primary textbook 2: *An Introduction to Mass and Heat Transfer*, by Stanley Middleman, Chapters 2-4, 6, 9-13
- Supplemental textbook (optional): *Introductory Transport Phenomena,* by R.B. Bird, W.E. Stewart, E.N. Lightfoot, and D.J. Klingenberg

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.

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:

Professionalism	7.5% (attendance, participation, etc).
Homework (~9-10 total)	32.5%
Two midterms	40% (20% each)
Final exam	20%
Total	100%

Homework will be due on Fridays 11:59 PM. *Students should upload their homework on Gradescope, which is linked in the course Brightspace webpage*. Unless specified by the instructor, the latest a homework can be turned in is two days past the due date (Sun 11:59 PM). Late homework will lose 20% off its maximum score for each day tardy. Homework after Sun 11:59 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 on the following dates and times.

- Tues, March 5, 8:00 – 10:00 PM, HAMP 3144
- Mon, April 8, 8:00 – 10:00 PM, HAMP 3144

The final exam will happen in the last week of the semester (April 29 – May 4). 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 Prof. 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 (subject to change)

Part I: Heat and mass transfer (~6 weeks). *Chapters 1-5 in Deen, Chapters 2-4, 10-11 in Middleman*

Lecture 1	Introduction to vector calculus – vectors, tensors, and divergence theorem (Deen Appendix) Balance laws for heat and mass transfer – introduction to fluxes (Deen Ch 1, Deen Ch 2, Middleman Ch 3.1, 11.2)
Lecture 2	Introduction to Fourier's/Fick's law. (Middleman 10.1) Boundary conditions and heat transfer coefficients. (Deen Ch 1, Deen Ch 2, Middleman Ch 3.2 (pg 42-43), 10.1 – 10.2)
Lecture 3	Heat transfer in composite solids -- series and parallel resistances (Middleman Ch 10.2) Introduction to Biot number. Reduction in dimensionality ad scaling (Deen Ch 3.4.1)
Lecture 4	Finish up discussion on Biot number (Deen Ch 3.4.1) Heat transfer in fins (Middleman Ch 10.3)
Lecture 5	1D problems – reaction diffusion systems. Introduction to Damkoler number, spherical catalyst (Deen Ch 3.2, Middleman Ch 3.2) Introduction to diffusion in gases (pseudo-binary approximation) (Middleman Ch 2.1.1, 2.1.2)
Lecture 6	Continue discussion on diffusion in gases (Middleman Ch 2.1) Pseudo steady-state approx. (Deen Ch 3.5, Middleman 2.1.3, 2.4, 11.1.1)
Lecture 7	Continue discussion of pseudo steady state
Lecture 8-9	Similarity solutions for heat/mass transfer problems (Deen Ch 4.2, Middleman Ch 11.3, 4.2, 4.3)
Lectures 10-11	Solution to transient heat/mass transfer (Deen Ch 5 for separation of variables, Middleman 11.1.2, 4.2, and 4.3 for chart solutions)
Lecture 12	Review problems

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

Lecture 13	Introduction to tensors Cauchy momentum equations (Deen Ch 6.2-6.3)
Lecture 14	Continuation of Cauchy momentum equations Introduction to stress tensor (Deen Ch 6.4)
Lecture 15	Continuation of stress tensor Hydrostatics (Deen Ch 6.6)

Lecture 16-17	Boundary conditions for flow and surface tension (BSL-K Ch 2.1) Example problem surface tension
--EXAM 1---	
Lecture 18	Unidirectional flows: Poiseuille and Couette flows (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 (Deen Ch 9.1-9.2)
Lecture 22	Review (if necessary)

Part III: Applications (~3 weeks). *Chapter 9 in Deen, Chapters 6, 8, 12, 13 in Middleman*

Lecture 23	Momentum boundary layers (concepts). Scaling of boundary layer (Deen Ch 8) Introduction to friction factors (BSL-K Ch 6, Middleman Ch 6.1, 12.1)
---EXAM 2---	
Lecture 24-25	Convective heat and mass transfer. Introduction, boundary layer, Sherwood/Nusselt numbers (Deen Ch 9, Deen Ch 10, Middleman Ch 6.1, 12.1) Estimating heat and mass transfer coefficients via correlations (Middleman Ch 12.2, 12.3, 6.3)
Lectures 26-27	Macroscopic mass and energy balances (BSL-K Ch 7, Ch 11). Heat exchangers (Middleman Ch 13)
Lecture 28	Other examples of macroscopic balance: dialysis, or friction loss in pipes, etc. (BSL-K Ex 23.1-3, Middleman Ch 8)
Lectures 29-30	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 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.

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.

PURDUE UNIVERSITY

ChE 554: Smart Manufacturing in the Process Industries

Course Information

- **ChE 554: Smart Manufacturing in the Process Industries**
- **CRN:** 18317/18322
- **Instructional Modality**: *Asynchronous-Online*
- **Meeting day(s) and time(s)**. *This course starts on January 8 and runs until April 27.* 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.edu
    - **Office** Location: FRNY
    - **Office Number:** G027C
- **Professor G V Reklaitis**
    - **Email:** reklaiti@purdue.edu
    - **Office** Location: FRNY
    - **Office 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.**
  - There will be readings available within Brightspace.
- **Software**
  - MatLab (which can be accessed via ECN). For more information about accessing Matlab, click **here.**
  - We will also be analyzing data using “Anaconda,” (a popular Python distribution), click **here** to learn more about how to download it and get started.
- **Hardware requirements**
  - A laptop that can connect to the internet and run the **Microsoft Office Suite** (available free to all Purdue Students)
- **Brightspace learning management system**
  - 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%
		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: 82.5%-85.49%
B-: 79.5%-82.49%
C+: 76.5%-79.49%
C: 72.5%-75.49%
C-: 69.5%-72.49%
D+: 66.5%-69.49%
D: 62.5%-65.49%
D-: 59.5%-62.49%
F: 49.4%-below

Academic Integrity

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: drc@purdue.edu 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 AI 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

* 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 WellTrack**.** 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 Office of the Dean of Students. 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 Purdue Wellness Coach at RecWell. 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 evans240@purdue.edu.

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 Counseling and Psychological Services (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.

CHE 597: Computational Optimization, Spring 2024

Instructor: Can Li
Email: canli@purdue.edu
Classroom: Hampton Hall of Civil Engineering, Room 2102
Time: Tuesday and Thursday, 4:30 pm - 5:45 pm
Office: Forney Hall of Chemical Engineering, Room G027A
Office Hours: Thursday, 3:30 pm - 4:30 pm
Make-up lecture classroom Max W and Maileen Brown Family Hall (BHEE) 234
Make-up lecture time Wednesday, 4:30 pm - 5:45 pm

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.

Syllabus

Date	Topic	Slides	Homework
Tue Jan 9	Introduction to Course	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%201/Lecture_1_Intro_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%201/Lecture_1_Intro_ipad.pdf)	HW1 (https://github Computational-Opti
Thu Jan 11	Convex sets, functions	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%202/Lecture_2_convex_sets_and_functions_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%202/Lecture_2_convex_sets_and_functions_ipad.pdf)	
Tue Jan 16	Unconstrained optimization	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%203/Lecture_3_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%203/Lecture_3_ipad.pdf)	HW2 (https://github Computational-Opti
Thu Jan 18	Linear Programming Applications	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%204/Lecture_4_Linear_Programming_Applications_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%204/Lecture_4_Linear_Programming_Applications_ipad.pdf)	
Tue Jan 23	Polyhedron Theory	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%205/Lecture_5_Polyhedron_Theory_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%205/Lecture_5_Polyhedron_Theory_ipad.pdf)	HW3 (https://github Computational-Opti
Thu Jan 25	Simplex Algorithm	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%206/Lecture_6_Simplex_Algorithm.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%206/Lecture_6_Simplex_Algorithm_ipad.pdf)	
Tue Jan 30	Linear Programming Duality	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%207/Lecture_7_Linear_Programming_Duality_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%207/Lecture_7_Linear_Programming_Duality_ipad.pdf)	HW4 (https://github Computational-Opti
Thu Feb 1	Conic Programming	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%208/Lecture_8_Conic_Programming_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%208/Lecture_8_Conic_Programming_ipad.pdf)	
Tue Feb 6	Langrangian Dual and Optimality Conditions	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%209/Lecture_9_Langrangian_Dual_and_Optimality_Conditions_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%209/Lecture_9_Langrangian_Dual_and_Optimality_Conditions_ipad.pdf)	HW5 (https://github Computational-Opti
Thu Feb 8	Nonlinear Programming Algorithms	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2010/Lecture_10_Nonlinear_Programming_Algorithms_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2010/Lecture_10_Nonlinear_Programming_Algorithms_ipad.pdf)	
Tue Feb 13	Modeling of Discrete and Continuous Decisions	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2011/Lecture_11_Modeling_of_Discrete_and_Continuous_Decisions_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2011/Lecture_11_Modeling_of_Discrete_and_Continuous_Decisions_ipad.pdf)	HW6 (https://github Computational-Opti

Date	Topic	Slides	Homework
Thu Feb 16	Formulating Mixed-Integer Linear Programming Models	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2012/Lecture_12_Formulating_Mixed_Integer_Linear_Programming_Models_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2012/Lecture_12_Formulating_Mixed_Integer_Linear_Programming_Models_ipad.pdf)	
Tue Feb 20	Mixed-Integer Linear Programming Applications	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2013/Lecture_13_Mixed_Integer_Linear_Programming_Applications_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2013/Lecture_13_Mixed_Integer_Linear_Programming_Applications_ipad.pdf)	HW7 (https://github Computational-Opti
Thu Feb 22	Branch and Bound	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2014/Lecture_14_Branch_and_Bound_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2014/Lecture_14_Branch_and_Bound_ipad.pdf)	
Tue Feb 27	Cutting Planes	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2015/Lecture_15_Cutting_Planes_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2015/Lecture_15_Cutting_Planes_ipad.pdf)	
Thu Feb 29	Midterm Review	practice exam solution (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Practice%20Exam%201/Practice_Exam_1_ChE_597_2024_Spring_solution.pdf)	
Thu Mar 7	Nonconvex Optimization Applications	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2016/Lecture_16_Nonconvex_Optimization_Applications_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2016/Lecture_16_Nonconvex_Optimization_Applications_ipad.pdf)	HW8 (https://github Computational-Opti
Tue Mar 19	Convex Relaxations	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2017/Lecture_17_Convex_Relaxations_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2017/Lecture_17_Convex_Relaxations_ipad.pdf)	
Thu Mar 21	Branch and Reduce	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2018/Lecture_18_Branch_and_Reduce_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2018/Lecture_18_Branch_and_Reduce_ipad.pdf)	HW9 (https://github Computational-Optimization/blob/r
Tue Mar 26	Decomposition Algorithms for MINLP	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2019/Lecture_19_Decomposition_Algorithms_for_MINLP_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2019/Lecture_19_Decomposition_Algorithms_for_MINLP_ipad.pdf)	
Thu Mar 28	Stochastic Programming and Benders Decomposition	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2020/Lecture_20_Stochastic_Programming_and_Benders_Decomposition_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2020/Lecture_20_Stochastic_Programming_and_Benders_Decomposition_ipad.pdf)	HW10 (https://githu Computational-Opti
Tue Apr 2	Column Generation and Dantzig Wolfe Decomposition	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2021/Lecture_21_Column_Generation_and_Dantzig_Wolfe_Decomposition_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2021/Lecture_21_Column_Generation_and_Dantzig_Wolfe_Decomposition_ipad.pdf)	
Thu Apr 4	Course Project	slides () ipad ()	
Tue Apr 9	Lagrangian Relaxation and Decomposition	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2022/Lecture_22_Lagrangian_Relaxation_and_Decomposition_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2022/Lecture_22_Lagrangian_Relaxation_and_Decomposition_ipad.pdf)	HW 11 (https://githu Computational-Opti
Thu Apr 11	Augmented Lagrangian and ADMM	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2023/Lecture_23_Augmented_Lagrangian_and_ADMM_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2023/Lecture_23_Augmented_Lagrangian_and_ADMM_ipad.pdf)	
Tue Apr 16	Bilevel Optimization	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2024/Lecture_24_Bilevel_Optimization_slides.pdf) ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2024/Lecture_24_Bilevel_Optimization_ipad.pdf)	
Thu Apr 18	MIP Solvers	slides (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Lecture%2025/Lecture_25_MIP_Solvers.pdf)	HW 12 (https://githu Computational-Opti
Tue Apr 23	Project Consulting		

Date	Topic	Slides	Homework
Thu Apr 25	Final Review	ipad (https://github.com/li-group/ChE-597-Computational-Optimization/blob/main/Practice%20Exam%202/Practice_Exam_2_ChE_597_2024_Spring_soln.pdf)	

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. 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 (2014). Integer programming. Graduate Texts in Mathematics
6. Boyd, S. P., & Vandenberghe, L. (2004). Convex optimization. Cambridge university press.
7. Tawarmalani, M., & Sahinidis, N. V. (2013). Convexification and global optimization in continuous and mixed-integer nonlinear programming: theory, algorithms, software, and applications (Vol. 65). Springer Science & Business Media.
8. Horst, R., & Tuy, H. (2013). Global optimization: Deterministic approaches. Springer Science & Business Media.

Software

We will use the following software

- Pyomo (https://www.pyomo.org/) is a collection of Python software packages for formulating optimization models. Tutorial: ND Pyomo Cookbook (https://jckantor.github.io/ND-Pyomo-Cookbook/README.html)
- Gurobi (https://www.gurobi.com/documentation/) and Cplex (https://www.ibm.com/products/ilog-cplex-optimization-studio) are both high-performance mathematical programming solver for linear programming, mixed integer programming, and quadratic programming.
- Mosek (https://www.mosek.com/) 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.
- Pytorch (https://pytorch.org/) PyTorch is a machine learning framework based on the Torch library, used for applications such as computer vision and natural language processing, originally developed by Meta AI and now part of the Linux Foundation umbrella.

Prerequisite

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

- YouTube videos review of linear algebra and calculus by 3Blue1Brown (https://www.youtube.com/@3blue1brown/courses)
- Linear algebra review (https://www.cs.cmu.edu/~zkolter/course/linalg/index.html) videos by Zico Kolter
- General mathematical review: Appendix A of Boyd and Vandenberghe (2004) (https://web.stanford.edu/~boyd/cvxbook/bv_cvxbook.pdf)

Related courses

- Convex optimization (https://www.stat.cmu.edu/~ryantibs/convexopt/) by Ryan Tibshirani
- Convex analysis (https://ocw.mit.edu/courses/6-253-convex-analysis-and-optimization-spring-2012/pages/syllabus/) by Dimitri Bertsekas
- Linear programming (https://www2.isye.gatech.edu/~sdey30/CourseLinearProgramming.html) by Santanu Dey
- Integer programming (https://coral.ise.lehigh.edu/~ted/teaching/ie418/) by Ted Ralphs
- Linear and convex optimization classes (https://www2.isye.gatech.edu/~nemirovs/) by Arkadi Nemirovski

Contact:
Purdue University
610 Purdue Mall
West Lafayette
IN, 47907, USA
(Maps (https://goo.gl/maps/37FPbUkUgS59Xnec9))
Follow us:
(https://twitter.com/Can__Li) (https://scholar.google.com/citations?user=EkwNNlAAAAAJ&hl=en) (https://www.linkedin.com/in/can-li-b36647a4/) (https://github.com/li-group) (https://www.youtube.com/channel/UCxuFcGhbr50bVaDPo4CECbA)

Crystallization Systems Engineering

Aim

To provide an introduction to advanced concepts of crystallization process engineering, including crystallization mechanisms, multicomponent crystallization and crystallization in impure media, as well as population balance modeling, model-based dynamic optimization and control, process analytical technology (PAT) and chemometrics and quality-by-design techniques. Introduce students in approaches and tools for the mathematical modeling and control of crystallization systems and to provide hands on experience with simulation software packages as well as a variety of PAT technologies.

Learning Outcomes

On completion of the training, the students are expected to be able to:

- Understand the fundamentals of crystallization thermodynamics and kinetics.
- Understand key concepts of crystallization technologies and control approaches
- Understand key differences between batch and continuous crystallization technologies
- Understand the key features and develop practical experience in the use of process analytical technologies such as ATR-UV/Vis, FBRM, Raman and Image analysis for monitoring crystallization processes
- Understand the main numerical solution techniques for population balance models
- Implement in Matlab and apply direct numerical optimization techniques for optimal control, model predictive control and parameter estimation
- Formulate mathematical models, develop dynamic simulations and optimization as well as parameter estimation based on experimental data for batch and continuous crystallization processes using Matlab as well as dedicated simulation software packages.
- Industrial case studies of crystallization process development delivered by a series of industrial guest lecturers.

Content

Particulate crystal characteristics; crystal size distribution, shape, purity, polymorphism. Crystallization mechanisms, nucleation, growth, breakage, agglomeration, effect of additives on growth and nucleation. Description of phase diagram and supersaturation. Analysis and conceptual design of crystallization processes in the phase diagram. Multicomponent crystallization and phase diagrams. Crystallization technologies (cooling, antisolvent, reactive, evaporative, membrane, microfluidic, melt, etc.). Overview of batch and continuous crystallization technologies and unit operations. Fluid dynamics in solid-liquid systems, scale-up. Crystallization in high share.

Process analytical technologies, quality-by-design and design space. Presentation of key process analytical tools used for monitoring and control of crystallizations processes (FBRM, ATR-UV/Vis/FTIR, Raman, ultrasound, image analysis based approaches, acoustic monitoring), and calibration procedures. Signal processing, sensor integration and crystallization process informatics system.

Model-free design and control approaches. Supersaturation control, direct design and direct nucleation control and applications.

Model-based optimization and control approaches. Population balance modeling (one- and multidimensional), with solution approaches (method of moments, quadrature method of moment, method of classes, finite difference, method of characteristics). PBM for modeling CSD, shape distribution and polymorphic transformation. Dynamic modeling of batch and continuous (batch and plug flow) crystallization systems. Dynamic optimization and optimal control using direct numerical optimization (control vector parameterization, simultaneous strategies and multiple shooting). Parameter estimation, and robust optimization. State and parameter estimation and nonlinear model predictive control for crystallization processes. Applications to batch, continuous mixed suspension mixed product removal (MSMPR), cascade of MSMPR and plug flow crystallization processes.

Industrial case studies for crystallization development delivered by a series of industrial guest lecturers.

Simulation studies using Matlab and gCrystal, and CrySiV. Industrial case studies.

Delivery-mode:

Lecture (L), Computing Laboratory (CL), Practical Study Observation (PSO) and laboratory session.

Assessment:

- Assignemnt 1 (group) 25%: Short paper based on laboratory experiment.
- Assigment 2 (individual) 30%: Short paper based on simulation exercise.
- Assignment 3 (individual) 20%: PBM homework
- Assignment 4 (individual) 25%: Set of HW assignments

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:	bmtacket@purdue.edu
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***; 2nd ed. 2001, or **3rd 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***; 3rd ed. 2004.
- Bockris, J. O’M.; Reddy, A. K. N. ***Modern Electrochemistry, Vol 1, Vol 2a, Vol 2b***; 2nd ed 2000. (available in pdf online from Springer).
- Pletcher, D. ***A First Course in Electrode Processes****;* 2nd ed. 2009.

Technology Requirement: MS Office

Purdue University
CHE 597 Industrial Chemical Technology
Fall 2024, Tue-Thu 1:30-2:45, FRNY 1043

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):

Tue 20 Aug	Course introduction; scope of the chemical and allied process industries
Thu 22 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 27 Aug	Natural Products 1 - Animal and vegetable fiber, leather, oils, fats, waxes, gelatin, dairy products, food processing
Thu 29 Aug	Natural Products 2 - Pulp and paper, naval stores, resins, turpentine, rosin, rubber (Report 1 Due)
Tue 3 Sep	Inorganics 1 - Chemistry of dehydration/hydration: ceramic pottery, tile, and brick, glass, plaster, cement, mortar, and concrete
Thu 5 Sep	Inorganics 2 - Chemistry of reduction: ore smelting, iron and steel, silicon, copper, brass, bronze, aluminum

Tue 10 Sep	Inorganics 3 - Bases and acids: soda ash, caustic soda, lime, mineral acids (nitric, sulfuric, phosphoric, hydrochloric)
Thu 12 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 17 Sep	Fuels 1 - Wood, coal, petroleum (gasoline, diesel, jet fuel, fuel oil), LPG, natural gas
Thu 19 Sep	Fuels 2 - Natural gas processing, petroleum refining processes and products
Tue 24 Sep	Fuels 3 - Synthetic fuels: town gas, F-T, SNG, MTG, biofuels
Thu 26 Sep	Organics 1 - Wood and coal chemicals and materials (Report 3 Due)
Tue 1 Oct	Organics 2 - Basic building blocks: acetylene, olefins (ethylene, propylene, butadiene) aromatics (BTX, Styrene), carbon monoxide
Thu 3 Oct	Organics 3 - Commodity intermediates and solvents: alcohols glycols and phenols, aldehydes and ketones, acids, esters, ethers
Tue 8 Oct	No Class - Fall Break
Thu 10 Oct	Organics 4 - Commodity monomers and polymers (PE, PP, PS, PET, PC, SBR) (Report 4 Due)
Tue 15 Oct	Organics 5 - Adhesives, coatings, films, fibers, plastics
Thu 17 Oct	Organics 6 - Fine chemicals: dyes pigments and cosmetics, flavors and fragrances, soap and detergents, explosives, agrichemicals, pharmaceuticals
Tue 22 Oct	Organics 6 continued
Thu 24 Oct	Organics 7 - Fermentation and biochemical processes; biotechnology (Report 5 Due)
Tue 29 Oct	Possible No Class -AIChE Meeting
Thu 31 Oct	Technical Impact Factor 1 - Homogeneous and heterogeneous catalysis
Tue 5 Nov	Technical Impact Factor 2 - Engineering and operational digital computation
Thu 7 Nov	Current Issues 1 - Environmental protection: air, wastewater, land; personnel protection: health and safety (Report 6 Due)
Tue 12 Nov	Current Issues 2 - Loss prevention and process safety
Thu 14Nov	Current Issues 3 - Sustainability: triple bottom line, life cycle analysis, industrial ecology, green chemistry and engineering
Tue 19 Nov	Current Issues 4 - Sustainability: population and economic growth, raw materials and energy demands
Thu 21 Nov	Current Issues 5 - Climate change
Tue 26 Nov	Current Issues 6 - Carbon dioxide management, capture, and sequestration
Thu 28 Nov	Thanksgiving Break
Tue 3 Dec	Current Issues 7 - Impact of shale gas and oil (Report 7 Due; Bonus Report Due)
Thu 5 Dec	No Class

Homework Reports:

Report 1 - Industry Structure and Statistics (Due 29 August)
Report 2 - Reaction Path Synthesis: Solvay Process (Due 12 September)
Report 3 - Block Flow Diagram: Petroleum Refining (Due 26 September)
Report 4 - Process Supply Chain: Polyethylene Terephthalate (Due 10 October)

Report 5 - General Purpose Batch Processing: Fine Chemical Manufacture (Due 24 October)
Report 6 - Safety and Environmental Protection: Methyl Isocyanate (Due 7 November)
Report 7 - Sustainability: Carbon Management (Due 3 December)
Bonus Report: Process Narrative: Major Chemical Intermediate (Due 3 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 drc@purdue.edu 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 (5th Ed and On-line, Wiley)
Ullmann's Encyclopedia of Industrial Chemistry (5th Ed and On-line, Wiley)
Shreve's Chemical Process Industries (5th Ed, McGraw-Hill Special Reprint Edition)
Handbook of Chemical Technology and Pollution Control (Robert Myers, 3rd Ed, Elsevier)
Handbook of Petroleum Refining Processes (Martin Hocking, 2nd 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: 1-882615-92-1
- *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 5
Homework 2: due February 26
Homework 3: due April 1
Homework 4: due April 22
Presentation 1: Feb 29 (8-10 PM)
Presentation 2: April 15 (8-10 PM)
Final Report due: April 28

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 9: Introduction
- January 11: Physiology overview (I)
- January 16: Physiology overview (I)
- January 18: Physiology overview (III)
- January 23: Interactions of blood with biomaterials (I)
- January 25: Interactions of blood with biomaterials (II)
- January 30: Kidney structure/function
- February 1: Normal kidney function
- February 6: Chronic kidney disease (CKD) and end-stage renal disease (ESRD)
- February 8: Uremic toxins: Chemical structure and clinical relevance
- February 13: Hemodialysis membrane properties
- February 15: Hemodialysis mass transfer
- February 20: Hemodialysis dose: Mass balance principles
- February 22: Extracorporeal therapy for AKI
- February 27: New device approaches for ESRD and AKI
- February 29: Extracorporeal therapies beyond renal failure
- **February 29 (8-10 PM): Presentation #1**
- March 5: No class
- March 7: No class
- March 12: Spring Break
- March 14: Spring Break
- March 19: Drug/device combinations*
- March 21: Wearable devices*
- March 26: Vascular access for dialysis
- March 28: Medical device regulation and clinical trials (I)
- April 2: Medical device regulation and clinical trials (II)
- April 4: Medical device market dynamics
- April 9: Medical device product development: Design verification/validation (I)
- April 11: Medical device product development: Design verification/validation (II)
- **April 15 (8-10 PM): Presentation #2**
- April 16: Medical device product development: Process Validation (I)
- April 18: Medical device product development: Process Validation (II)
- April 23: Applying risk analysis to device design (I)
- April 25: Lean manufacturing in the medical device industry, project management & regulatory strategy

*: guest lecture

K. Consulting with the Instructor. I encourage you to discuss academic or personal questions with me during my office hours or via email. These discussions need not be limited to CHE 59700 content.

L. Instructor's 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 I am unable to keep them; 4) provide a suitable guest lecturer when I am traveling; and 5) grade uniformly and consistently to the posted guidelines.

M. 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.**

N. 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.

O. 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.

P. 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.

Q. 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 Clark privately to discuss specific needs.

R. 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 Clark privately to discuss his/her specific needs. If you are a student with any form of individual learning needs, please speak with the faculty instructors 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.

S. 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. The evacuation and shelter-in-place procedures for the Mechanical Engineering building are posted at the entrances to all classrooms and detailed in the Building Emergency Plan (https://www.purdue.edu/ehps/emergency-preparedness/emergency-plans/bep/building-beps/me-bep.html). Students are responsible for understanding and adhering to these procedures in the event of an emergency. Please see additional information on Brightspace.

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 area of Purdue Mall outside 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.
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.

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. ***You are expected to check your @purdue.edu email address frequently.***

T. Use of Copyrighted Material. 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. 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.

CHE 59700 **Spring 2025**

Introduction to the Upstream Oil and Gas Industry

A. **Instructors.** Leon Robert, PhD and Nate Schultheiss, PhD

B. **Course Description.** This course provides a practical overview of current engineering technologies and practices to identify, drill and complete hydrocarbon bearing reservoirs. The oil and gas (O&G) industry seeks to achieve long-term energy security with a balanced, diversified, and sustained investment in both traditional energy sources and lower-emission solutions throughout the energy transition in this century. Access to reliable and affordable energy is essential to our daily lives and is a major underpinning of social and economic progress in the U.S. This course incorporates practical examples and applications to progressively give the student an introduction to advanced knowledge of upstream O&G exploration and production.

This course is relevant to a broad base of students in engineering, geology, and chemistry, especially those planning a career in energy or more specifically in the oil and gas industry. The course content is designed especially for those students interested in upstream oil and gas topics including but not limited to exploration, drilling, production, hydraulic fracturing, and recent advances in each.

C. **Course Requirements**. ChE 20500 – Chemical Engineering Calculations or equivalent course is recommended by not mandatory.

D. **Instructor Biographical Information**.

- Leon Robert holds dual academic appointments at Purdue University as Professor of Engineering Practice in the Davidson School of Chemical Engineering and Professor of Clinical Practice in the Department of Entomology. He is a retired military officer and Professor Emeritus, United States Military Academy. He received his PhD in Entomology at Texas A&M University. In addition, he received B.A. and M.Ed. degrees from the State University of New York at Potsdam; an M.S. degree in Biology at Old Dominion University, and a M.S.S. degree from the U. S. Army War College. Recently he worked as a consultant for Chevron for 5 ½ years in drilling and completions operations in the Permian Basin of West Texas and Southern New Mexico.

- Nate Schultheiss is the Director of Unconventional Energy at Purdue University where he shares his time between the Davidson School of Chemical Engineering and Pioneer Oil Company (Vincennes, IN). Pioneer Oil is one of the largest O&G operators in the Illinois Basin. Part of his responsibilities are to direct Purdue's Enhanced Oil Recovery laboratory where fundamental and applied research is conducted to maximize hydrocarbon production for O&G operators. Before joining Purdue University, Nate was a technology leader at Halliburton guiding the research and development of chemical solutions used in completions operations. As a chemical subject matter expert, he supported Halliburton's field operations in the piloting of new products and services. He received his PhD in Chemistry at Kansas State University. In addition, he received B.S. and M.S. degrees from Missouri State University also in Chemistry.

E. Required and Recommended Textbooks.

- **No** required textbooks for this course, but topical articles will be provided throughout the course for reading/understanding.

F. Course Learning Objectives.

- Describe the history of the oil and gas industry.
- Identify the geological origins of petroleum reservoirs and reservoir fluids.
- Describe the components and processes involved in the drilling, completion, and production of oil and gas reservoirs.
- Explain exploration, production, and operations concepts associated with the oil and gas industry.
- Demonstrate and apply terminology and skills necessary to gain employment in the oil and gas industry.
- Demonstrate an understanding of safety and compliance standards and regulations applicable to onshore upstream production and completions.
- Discuss the role of environmental stewardship in the petroleum engineering profession.

G. Course Meeting Schedule.

Lectures:	Monday/Wednesday/Friday time/location TBD
Quizzes:	January 31, February 17, March 3, April 2, and April 23
Individual Project Selected:	by March 7
Individual Project due:	May 7

At the approximate mid-point in the semester students will choose an individual topic related to oil and gas production engineering or technology. Topic will be described in 1-3 sentences and emailed to instructor for approval. Upon approval, a completed written report, not to exceed five double-spaced pages will be due at the end of the semester in lieu of a final exam.

On March 7th, additional information will be provided about the Individual Project requirements.

H. Instructor Contact Information.

- Professor Leon Robert – Email: Robert9@purdue.edu; Telephone: (765) 494-0551 (office), (806)342-5020 (cell)
  Office: FRNY 2043B
  Office Hours: TBD

- Dr. Nate Schultheiss – Email: Nschulth@purdue.edu; Telephone: (765) 586-4382 (cell)
  Office: FLEX 2041C
  Office Hours: TBD

I. Assessment of Course Outcomes.

A weighted grade average will be calculated as follows.

- Five (5) Quizzes – 50% of total

  Quiz #1: January 31
  Quiz #2: February 17
  Quiz #3: March 3
  Quiz #3: April 2
  Quiz #4: April 23

- Individual Project – 50% of total

  Due: May 7

- **Grading Scale**

  A: 100% - 90% of the weighted points
  B: 89.9% - 80% of the weighted points
  C: 79.9% - 70% of the weighted points
  D: 69.9% - 60% of the weighted points
  F: Less than 60% of the weighted points

J. Course Schedule.

Lecture	**Date**	**Topic**
BLOCK 1 – Introduction to Hydrocarbons and the Oil and Gas Industry		
Lecture 1	Jan 13	A Brief History of the Oil and Gas Industry in the U.S.
Lecture 2	Jan 15	Origin and Occurrence of Hydrocarbons
Lecture 3	Jan 17	Reservoir Engineering – Rock and Fluid Properties
No Class	Jan 20	**MLK Day – University Closed**
Lecture 4	Jan22	Petroleum Geology
Lecture 5	Jan 24	Petroleum Exploration

Lecture 6	Jan 27	Procuring the Right to Drill: Mineral Rights and Leasing
Lecture 7	Jan 29	Regulatory Permits
BLOCK 2 – Drilling Rig Systems and the Drilling Process		
Lecture 8	Jan 31	**Quiz #1 (Block 1)** & Introduction to the Drilling Rig and Rig Site
Lecture 9	Feb 3	Well Design
Lecture 10	Feb 5	Drilling Fluids and Chemicals
Lecture 11	Feb 7	Basic Drilling Operations
Lecture 12	Feb 10	Well Flowback Fluids and Tailings
Lecture 13	Feb 12	Well Bore Architecture
Lecture 14	Feb 14	Introduction to Gas and Liquid Flow Through Well Tubing
Lecture 15	Feb 17	**Quiz #2 (Block 2)** Open Hole Evaluation using Well Logs, Cores, and Fluid Tests
Lecture 16	Feb 19	Well Casing (Liner Completion)
Lecture 17	Feb 21	The Cementing Process
Lecture 18	Feb 24	Well Control
Lecture 19	Feb 26	Well Control Calculations
Lecture 20	Feb 28	Drilling Safety
BLOCK 3 – Gas production and Completions Operations		
Lecture 21	Mar 3	**Quiz #3 (Block 2)** & Shale Gas
Lecture 22	Mar 5	Introduction to Completions Operations
Lecture 23	Mar 7	**Project Topic Selection** & Perforations
Lecture 24	Mar 10	Hydraulic Fracturing Operations
Lecture 25	Mar 12	Chemistry of Fracturing Fluids
Lecture 26	Mar 14	Oil and Gas Field Processing Basics
No Classes	**Mar 17-21**	**Spring Break**
Lecture 27	Mar 24	Pollution Prevention
Lecture 28	Mar 26	Emergency Planning and Environmental Law
Lecture 29	Mar 28	Gas Dehydrators and Separators
Lecture 30	Mar 31	Gas Compressors and Water Disposal
Block 4 – Well Intervention and Technology Advancements		
Lecture 31	Apr 2	**Quiz #4 (Block 3)** & Storage Tanks and Work Over Techniques
Lecture 32	Apr 4	Supervision and Management of an Oil and Gas Site
Lecture 33	Apr 7	Technology Advancements Part 1 (Exploration)
Lecture 34	Apr 9	Technology Advancements Part 2 (Drilling)
Lecture 35	Apr 11	Technology Advancements Part 3 (Completions and Production)
Lecture 36	Apr 14	Enhanced Recovery Techniques (Secondary Production)
Lecture 37	Apr 16	Enhanced Recovery Techniques (Tertiary Production)
Lecture 38	Apr 18	Geothermal
Lecture 39	Apr 21	Improved Oil Recovery Methods: Water, CO2, and Chemical Flooding
BLOCK 5 – The Big Picture and Final Project		
Lecture 40	Apr 23	**Quiz #5 (Block 4)** & Oil and Gas Transportation – Trucks, Railway, Pipelines, and Ships
Lecture 41	Apr 25	Closing a Project – Plug and Abandonment and Site Restoration
Lecture 42	Apr 28	Global Best Practices

Lecture 43	Apr 30	Corporate Social Responsibility
-	May 2	Work on Individual Project
-	**May 7**	**Individual Project Due**
No Class	**May 5-10**	**Final Exams**

K. Consulting with the Instructor. I encourage you to discuss academic or personal questions with me during my office hours or via email. These discussions need not be limited to CHE 49700/50200 content.

L. Instructor's 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 I am unable to keep them; 4) provide a suitable guest lecturer when I am traveling; and 5) grade uniformly and consistently to the posted guidelines.

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P. 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 based on 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.

Q. Diversity and Inclusion Statement. In our discussions, structured and unstructured, we will explore a variety of challenging issues, which can help us enhance our understanding of different experiences and perspectives. This can be challenging, but in overcoming these challenges we find the greatest rewards. While we will design guidelines as a group, everyone should remember the following points:

- We are all in the process of learning about others and their experiences. Please speak with the instructors, anonymously if needed, if something has made you uncomfortable.
- Intention and impact are not always aligned, and we should respect the impact something may have on someone even if it was not the speaker's intention.
- We all come to the class with a variety of experiences and a range of expertise, we should respect these in others while critically examining them in ourselves.

R. Bereavement Policy. Purdue recognizes that a time of bereavement is 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 Clark privately to discuss specific needs.

S. Individual Learning and Testing Needs. Any student who feels he/she may need accommodation with any aspect of the course based on personal circumstances should contact Professor Clark privately to discuss his/her specific needs. If you are a student with any form of individual learning needs, please speak with the faculty instructors whether 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.

T. 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 goal of maintaining a safe and secure campus.
The following is a review of the emergency procedures at Purdue University. The evacuation and shelter-in-place procedures for Hampton Hall are posted at the entrances to all classrooms and detailed in the Building Emergency Plan (https://www.purdue.edu/ehps/emergency_preparedness/bep/HAMP-bep.html.) Students are responsible for understanding and adhering to these procedures in the event of an emergency. Please see additional information on Brightspace.

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 Hampton Hall (FRNY). 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.

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. ***You are expected to check your @purdue.edu email address frequently.***

U. Use of Copyrighted Material. 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. 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, 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.

V. Responsible Use of AI in Completing Coursework. Advancements in Artificial intelligence (AI) provide students with unparalleled access to information and problem-solving capabilities. However, with these advantages come the responsibilities of ethical use and academic integrity. This statement outlines the expectations and guidelines for the responsible use of AI in our course.

By adhering to these guidelines, students aim to:
- Uphold academic honesty and personal integrity.
- Ensure equitable access and opportunities for all students.
- Develop skills for critical thinking and independent reasoning.
- Understand the strengths and limitations of AI tools.

Guidelines for Responsible Use:

• Original Work: Students should ensure that assignments submitted are original and based on their understanding. While AI can assist in research or provide general guidance, it should not produce work on behalf of the student.

• Citation: Any content, ideas, or assistance obtained through AI tools must be appropriately cited, like any other reference or source. You will need to locate the relevant citations from the primary literature (i.e., journal articles).

• Collaboration: If a student collaborates with AI tools, (you are encouraged to do so in this course) they must specify the nature and extent of this collaboration in their submission. This includes providing details of the prompts used to generate the AI responses.

Prohibited Uses: AI should not be used to complete quizzes, reflections, presentations, projects, or any other assessments unless explicitly permitted by the instructor.

• Accessibility: All students must have equal access to AI tools. If a particular tool is used in a course, it should be free of cost for all users.

• Data Privacy: Students must be cautious when sharing personal or sensitive information with AI platforms and should be familiar with the terms of service of any third-party AI tools.

• Sharing of copyrighted material with third-party AI tools: This is prohibited. While faculty and instructors do not own copyright to facts or ideas in their discipline, they do own copyright to their expression, explanation, and presentation of those facts and ideas in course notes, PowerPoint slides, etc. including assessments constructed for the course. As such, those instructor-generated materials should never be uploaded to any third-party site (whether AI oriented or not).

FERPA and Privacy Issues: Both student and instructor commit to never sharing personally identifiable information about students with any third-party AI tool.

Consequences for Misuse:
Misuse of AI tools in coursework, which includes but is not limited to producing unoriginal work, uncited use of AI- generated content, or unauthorized assistance on assessments, will be considered a breach of academic integrity. Consequences will follow Purdue policy on academic dishonesty as detailed in this syllabus, which may include grade penalties, course failure, or more severe disciplinary actions.

The promise of AI in enhancing learning and research is vast, but it must be used judiciously. Responsible use not only ensures academic honesty but also maximizes genuine learning and skill development. Students are urged to approach AI as a supplementary tool, not a replacement for their unique intellectual capacities and insights.

W. **Netiquette.** Your instructor and fellow students wish to foster a safe online learning environment. All opinions and experiences, no matter how different or controversial they may be perceived, must be respected in the tolerant spirit of academic discourse. You are encouraged to comment, question, or critique an idea, but you are not to attack an individual. Our differences, some of which are outlined in the University's nondiscrimination statement below, will add richness to this learning experience. Please consider that sarcasm and humor can be misconstrued in online interactions and generate unintended disruptions. Working as a community of learners, we can build a polite and respectful course ambience.

Please read the Netiquette rules for this course:

- Do not dominate any discussion. Give other students the opportunity to join in the discussion.
- Do not use offensive language. Present ideas appropriately.
- Be cautious in using Internet language. For example, do not capitalize all letters since this suggests shouting.
- Avoid using vernacular and/or slang language. This could possibly lead to misinterpretation.
- Keep an "open mind" and be willing to express even your minority opinion.
- Think and edit before you push the "Send" button.
- Do not hesitate to ask for feedback.

X. **Course Evaluation.** During the last two weeks of the course, you will be provided with an opportunity to evaluate this course and your instructors. Purdue uses an online course evaluation system. You will receive an official email from evaluation administrators with a link to the online evaluation site. You will have up to two weeks to complete this evaluation. Your participation is an integral part of this course, and your feedback is vital to improving education at Purdue University.

The instructors strongly urge you to participate in the evaluation system and to provide them honest and constructive feedback about how they may improve the course in future offerings.

Disclaimer: This syllabus is subject to change. Students will be notified through Brightspace in the event of changes to the syllabus.

CHE 597 Course Syllabus, Spring 2025 (Preliminary)

Instructors: Dr. Enrico N. Martinez

G015 Forney Hall, 49-66998, marti309@purdue.edu

Office Hours: Wednesdays, 4:30-6:00 or stop by, anytime

Text Required: Demirel, Y. and Rosen, M. A., Sustainable Engineering, Process Intensification, Energy Analysis, Artificial Intelligence, CRC Press, 2023.

Recommended: Allen, D. T., and Shonnard, D. R., *Sustainable Engineering,* Pearson**,** 2012.

Course Outcomes

1) Apply principles of engineering, science, and mathematics to design sustainable products and processes
2) Apply sustainable chemical 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 sustainable 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.

Unit Level Objectives

Identify the details of the natural resource and environmental challenges that chemical engineers face in designing for sustainability.
Define the analysis and legislative frameworks for addressing environmental issues and sustainability
Identify and select the green and sustainable materials for an engineering design
Understand and apply the principles that chemical engineers can use to make their designs more sustainable
Understand and apply the tools that can be used to evaluate, and in some cases monetize, the benefits of more sustainable designs
Apply the principles and tools of sustainable design to particular cases encountered in the chemical process industry

Course Operation

- There will be three midterm exams during the semester; February 16, March 23 and April 20 (All in class).
- There will not be a final exam. The date scheduled for the final exam will be used to make up missed midterm exams.
- The final grade will be calculated considering Homework grades, Team Design Project Report and midterm exam grades.

Three One Hour Examinations (150 points each) .... 450 points
Individual Homework Assignments .... 150 points
Team Design Project .... 150 points
TOTAL .... 750 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	C- [at least]
60 – 69	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…)

Homework: Assignments will be loaded to Brightspace most Tuesday's and are due in completed form by the next Thursday, beginning of lecture. Late homework will be assessed a penalty of 5 pts if turned in by 4:30 PM. If not received by 4:30, 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 597) 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.

Suggested approach:
- Work all assigned problems individually.
- Meet with your study group to check your approach, your answers, and complete the solutions to the more difficult problems.
- Ask for help if these efforts have not been completely successful – don't approach a TA or your instructor with questions before you have done the above.
- Finally, prepare your own solution to submit.

We will grade selected problems and check that the other problems were attempted. Work in groups is encouraged, but you must submit your own solution with a list of names of your group members.
Any adjustments to homework grades should be handled with Professor Martinez or within one week after the assignment is returned. Solutions to all homework assignments, exams, and other handouts will be made available on the course Brightspace web site.

Exam Make-up Policy: Occasionally students may have to miss a midterm exam for personal or uncontrollable reasons. However, if an exam needs to be missed, there will NOT be a make-up 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, job interview) 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.

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 pts.

Design Project: There will be one design project at the end of the semester. The project will be done by teams of three students each. Further details of the project will be supplied after the spring break.

Course Contents

Introduction to Sustainability
Energy
Materials Use
Environmental emissions
Risk assessment
Risk-Based environmental law
Definition of Life-Cycle
Life-Cycle assessment
Life-Cycle-Based environmental law
Process-Based Life-Cycle assessments
Input-Output Life-Cycle Assessment
Hybrid approaches
Environmental law and regulation
Pollution prevention concepts and terminology
Environmental law and sustainability

Students are required to come the lectures prepared and will have to read the subject matter in advance, reading assignments will be included in the weekly homework statements.

Student Expectations.

This is a Three-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. I encourage you to take studying seriously and establish good study habits such as previewing the reading material ***before*** the lectures and practicing additional problems.

Instructors' Commitment.

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 we are unable to keep them; 4) provide a suitable guest lecturer when traveling; and 5) grade uniformly and consistently to the posted guidelines.

Consulting with the Instructor.

I encourage you to discuss academic or personal questions with us during our office hours or via email or Hotseat. These discussions need not be limited to ChE 59700 content.

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.**

Always remember the 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."

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.

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.

Attendance. University policy states that it is the responsibility of all students to attend all class sessions. You are expected to attend all lectures, labs and recitation periods. (http://www.purdue.edu/studentregulations/regulations_procedures/classes.html).

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.

Students should stay home and contact the Protect Purdue Health Center (496-INFO) if they feel ill, have any symptoms associated with COVID-19, or suspect they have been exposed to the virus. In the current context of COVID-19, in-person attendance will not be a factor in the final grades, but the student still needs to inform the instructor of any conflict that can be anticipated and will affect the submission of an assignment or the ability to take an exam. Only the instructor can excuse a student from a course requirement or responsibility. When conflicts can be anticipated, such as for many University-sponsored activities and religious observations, the student should inform the instructor of the situation as far in advance as possible. For unanticipated or emergency conflict, when advance notification to an instructor is not possible, the student should contact the instructor as soon as possible by email, through Brightspace, or by phone. 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, quarantine, or isolation, the student or the student's representative should contact the Office of the Dean of Students via email or phone at 765-494-1747. Our course Brightspace includes a link on Attendance and Grief Absence policies under the University Policies menu.

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 Martinez privately to discuss specific needs.

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.***

Individual Learning and Testing Needs.

Any student who feels he/she/they may need an accommodation with any aspect of the course based on a personal circumstance should contact Professors Martinez and Tackett privately to discuss his/her/their specific needs. If you are a student with any form of individual learning needs, please speak with the faculty instructors 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 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 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.
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.

The Protect Purdue Plan, which includes the Protect Purdue Pledge, is 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 (496-INFO) if you feel ill or know you have been exposed to the virus, properly wearing a mask in classrooms and campus building, at all times (e.g., mask covers nose and mouth, no eating/drinking in the classroom), disinfecting desk/workspace prior to and after use, maintaining appropriate social distancing with peers and instructors (including when entering/exiting classrooms), refraining from moving furniture, avoiding shared use of personal items, maintaining robust hygiene (e.g., handwashing, disposal of tissues) prior to, during and after class, and following all safety directions from the instructor.

Students who are not engaging in these behaviors (e.g., wearing a mask) will be offered the opportunity to comply. If non-compliance continues, possible results include instructors asking the student to leave class and instructors dismissing the whole class. Students who do not comply with the required health behaviors are violating the University Code of Conduct and will be reported to the Dean of Students Office with sanctions ranging from educational requirements to dismissal from the university.

Any student who has substantial reason to believe that another person in a campus room (e.g., classroom) is threatening the safety of others by not complying (e.g., not wearing a mask) may leave the room without consequence. The student is encouraged to report the behavior to and discuss next steps with their instructor. Students also have the option of reporting the behavior to the Office of the Student Rights and Responsibilities. See also Purdue University Bill of Student Rights.

MWF – 10:30 – 11:20 am

Instructor: Xiaoping Bao, Ph.D.
Office: FRNY 1158
Office Hours: By appointment as necessary
Contact: bao61@purdue.edu

Course Description and Goals
This course provides an introduction to the cutting-edge stem cell and immuno-engineering technologies. Stem cell-based regenerative medicine and immunotherapies are rapidly expanding research fields, and considerable hope is placed on the use of human stem cells in medicine to repair tissue for diseases that are currently incurable and treat cancers. **The objective of this course** is to provide students with the background, theory, and techniques of pluripotent stem cell engineering and immuno-engineering. Topics will include the generation of induced pluripotent stem cells, the directed differentiation of pluripotent stem cells, the genome editing of human pluripotent stem cells, RNA-seq analysis of the stem cells and their derivatives, disease modeling and therapies with stem cells, stem cell processing, biomaterials and 3D culture systems, and immune T and NK cell engineering for targeted cancer immunotherapies. It will also highlight the challenges during the translation of stem cell products from laboratory to clinics and opportunities for engineers and chemists. Students will also be trained on scientific literature search, writing and presentation.

Recommended (NOT REQUIRED) Texts
1. *Stem Cell Engineering: Principle and Practices*, David V. Schaffer, Joseph D. Bronzino and Donald R. Peterson, CRC Press, Inc., 2012, ISBN: 978-1439872048
2. *Developmental Biology*, Scott F. Gilbert and Michael J.F. Barresi, Sinauer, 2016, ISBN: 978-1-605-35470-5.

Grading
Participation (interactions with instructors)– 10%
Proposal – 40%
Presentation– 20%
Homework- 30%

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

Semester Manuscript/Proposal

Each student will be required to turn in **either** a review paper **or** proposal by the end of the semester (i.e., prior to 5p (Eastern) on **November 12, 2020**) regarding a topic within the realm of “stem cell engineering” of his/her choice.

For the review paper, the text of the document will include a review of the relevant literature and open discussion of future research that the student believes could lead to interesting results in the field. Exact details of the assignment will follow the format of Current Opinion in Chemical Engineering (see Guide for Authors: https://www.elsevier.com/journals/current-opinion-in-chemical-engineering/2211-3398/guide-for-authors), but the manuscript will not be longer than 8 pages (double-spaced, 12 point, Times New Roman font, with 1 inch margins), not including references. For the proposal, a paper formatted as an NIH grant proposal on stem cell engineering and regenerative medicine containing a one-page summary outlining the hypothesis and specific aims followed by a research strategy (8 pages single spaced) containing three sections: Significance, Innovation and Approach (see example in Brightspace). References are expected and are separate from the 8-page limit of the Research Strategy. The due date will be **November 12**.

Before beginning work on this manuscript, it is highly recommended that the student meet with the instructor in order to outline a planned topic of study. The presentation will be 20 minutes followed by 5-10 minutes of questions and will detail your grant proposal or review.

Week 1	**Tuesday, August 25** **Thursday, August 27**	Introduction: Genome, Cells, and Tissues
Week 2	Tuesday, September 1 Thursday, September 3	Mouse Embryonic Stem Cells, Gene Targeting and Transgenic Animals
Week 3	**Tuesday, September 8** **Thursday, September 10**	Regenerative Medicine: Human Embryonic Stem Cells
Week 4	Tuesday, September 15 Thursday, September 17	Directed Differentiation - 1
Week 5	**Tuesday, September 22** **Thursday, September 24**	Directed Differentiation - 2
Week 6	Tuesday, September 29 Thursday, October 1	Bioinformatives: RNA-seq and single cell RNA-seq
Week 7	**Tuesday, October 6** **Thursday, October 8**	Nuclear Transfer and Cellular Reprogramming
Week 8	Tuesday, October 13 Thursday, October 15	Induced Pluripotent Stem Cells and Disease Modeling
Week 9	**Tuesday, October 20** **Thursday, October 22**	Direct Reprogramming / Transdifferentiation
Week 10	Tuesday, October 27 Thursday, October 29	ZFN and TALEN Strategies for Genome Editing and Disease Modeling
Week 11	**Tuesday, November 3** **Thursday, November 5**	CRISPR/Cas9 Strategies for Genome Editing and Disease Modeling
Week 12	Tuesday, November 10 Thursday, November 12	CAR-T and NK Cells from Stem Cells
Week 13	**Tuesday, November 17** **Thursday, November 19**	Stem Cell Bioprocessing (maybe guest lecture) and Presentations
Week 14	Tuesday, November 24	
	Thursday, November 26	**Thanksgiving**
Week 15	**Tuesday, December 1** **Thursday, December 3**	Presentations
Week 16	Tuesday, December 8 Thursday, December 10	

CHE 59700-030 (3 credit-hours)
Financial Analysis and Project Management
Spring 2025

Class Location/ Format	FRNY B124 – In person
When	Monday, Wednesday, Friday 11:30p – 1:00p
Duration	January 13, 2025 – March 9, 2025
Exam Format	Interim and Final Presentations; Final Paper

Primary Instructor

Michelle Chutka
Email: mchutka@purdue.edu 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 19 years of experience in Medical Device industry, and has been performing consulting work after concluding her work as 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 2102 HAMP

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.

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 referenced 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 5th 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 (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 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	20%
Homework	20%
Mid-Point Presentation 1	20%
Final Presentation 2	20%
Final Paper	20%

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

***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 individually by each team member 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 2024 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 mchutka@purdue.edu. 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 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;
(iii) enabling other students to create work that is not their original work.

The consequence of the first offense of plagiarism is a grade of zero for the entire work, even if the work is a final presentation, final paper, or homework.

The consequence of the a second offense is an F mark for the class.

All students involved in the plagiarism will receive the above noted consequences, unless there is incontrovertible evidence that the original work that was plagiarized was done so without knowledge or permission from the original work's author.

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

NOTES: Instances in previous years have included students turning in overtly and obviously similar work. Where work is noted as required to be individual, students may collaborate on the problem-solving approach, but the write-up must be unique to each student. All involved students suspected of plagiarism or non-individual work will be given 0 points on the assignment regardless of who authored the "original" work.

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: http://www.purdue.edu/policies/academic-research-affairs/ia3.html

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:
http://www.purdue.edu/studentregulations/regulations_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:
http://www.purdue.edu/studentregulations/regulations_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:
https://www.purdue.edu/ehps/emergency_preparedness/

Students with Disabilities
Any academic accommodation must be arranged for by the student 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 www.purdue.edu/report-hate 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:
http://www.purdue.edu/purdue/ea_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 immediately **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 immediately 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 http://www.purdue.edu/ehps/emergency_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:
  - evacuation routes, exit points, and emergency assembly area
  - when and how to evacuate the building.
  - shelter in place procedures and locations
  - 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: http://www.purdue.edu/securePurdue/news/2010/emergency-preparedness-shots-fired-on-campus-video.cfm (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/

ChE 621: TRANSPORT PHENOMENA II
SPRING SEMESTER 2021

Lectures: MWF 3:30-4:20 **Location:** FRNY xxx/Zoom

Instructor: Prof. O. A. Basaran, FRNY 3060
765-494-4061 (phone); 765-494-0805 (fax); obasaran@purdue.edu

Teaching Assistant: NA

Course philosophy and objectives. Transport Phenomena II will deal with the analysis of transport of

- **momentum**
- **energy**
- **mass** and
- **electric charge**

in material media with emphasis on systems in which there are **density, temperature, concentration,** and **electric potential** gradients. Special emphasis will be placed in the course on stability of single- and multi-phase flows, interfacial mechanics, and electrically-driven flows and transport processes. Aside from focusing on transport phenomena, an equally important goal of the course is to expose the participants to mathematical methods that are applicable in diverse fields of science and engineering. These methods include linear stability analysis, select techniques from nonlinear dynamics, scaling concepts, and asymptotic analysis including regular and singular perturbation techniques.

Instructional method. We are fortunate to have two outstanding textbooks, one of which is required, to use in this course. Aside from these texts, there will also be extensive handouts of lecture notes and supplementary materials.

There will be weekly homework assignments (25% of the grade), two midsemester examinations during the semester (each worth 25% of the grade), and a final examination (also worth 25% of the grade). The midsemester exams may be of the take home type. Some years, a project or projects may be required or offered in lieu of the midsemester and/or the final exams. [*Dates for examinations will be announced with sufficient advanced notice during the semester.*]

Prerequisites. Class participants should be familiar with elementary vector and tensor analysis **at the minimum** at the level of undergraduate courses taught in mathematics departments and the Appendix on the subject that can be found in Bird, Stewart, and Lightfoot's *Transport Phenomena* (BSL) and **preferably** at the level of Aris's famous little book (Aris, R. 1962/1989 *Vectors, Tensors, and the Basic Equations of Fluid Mechanics.* Dover.) The students should also be at ease with certain rudiments of transport phenomena at or slightly above the level of BSL. A good background in calculus and ordinary differential equations is also essential.

Class attendance. Attendance at lectures, make up sessions, and optional sessions is optional, i.e. not required. All material that will be covered by Prof. Basaran during these meetings and that the students will be tested on can be found in the required text and the handouts. Thus, no new material is presented in any of the lectures or the other sessions.

Teaching evaluations. Student evaluations of the teaching and the course can provide useful inputs for improving the quality of the teaching and the content of the course in future years. Thus, students are strongly encouraged to submit on line evaluations of the course during the last week of classes.

Other logistical details. Participants will be provided additional handouts and/or may be referred to certain web sites for additional information that will be needed for proper administration of the course.

Required (1) and recommended (2) texts.

1. Deen, W. M. 2012 *Analysis of Transport Phenomena* (second edition). Oxford University Press. [**Required text.**]

2. Leal, L. G. 2007 *Advanced Transport Phenomena.* Cambridge University Press. [**Recommended but not required.**]

It also goes without saying that every serious graduate student should own copies of BSL and Aris. A list of additional supplementary or reference texts will be given out in class.

Homework assignments. Approximately once each week, homework will be assigned that addresses topics covered in lectures during that week (see the course outline below). Typically, one problem but sometimes a few problems will be selected (randomly) from each homework assignment for grading, i.e. if there are seven (7) problems in homework 3, we may grade one (1) problem, two (2) problems, or four (4) problems but never all seven (7) problems.

Course outline.

Week 1. Linear stability analysis. (Class notes.)

Week 2. Slightly nonlinear analysis and two-timing. (Class notes.) Review of Cartesian tensors and indicial notation. (First few chapters from Aris.)

Week 3. Transport equations, transport theorems, and boundary conditions. (Deen chapters 1-2.)

Week 4. Formulation, scaling and approximation techniques. (Deen chapter 3.)

Week 5. Similarity and (regular and singular) perturbation methods. (Deen chapter 4.)

Weeks 6 and 7. Solution methods for linear problems (especially FFTs). Motivation of methods by means of examples from transport phenomena as well as electricity and magnetism. Electrohydrodynamics. (Deen chapter 5. Melcher and Taylor 1969.)

Week 8. Review of: key concepts in fluid mechanics, interfacial mechanics and surface tension gradient-driven flows. (Deen chapter 6.)

Week 9. Unidirectional and nearly unidirectional flows, lubrication approximation, and heat and mass transfer analogs. (Deen chapter 7.)

Week 10. Creeping flows. (Deen chapter 8.)

Week 11. Laminar flows at high Reynolds number. (Deen chapter 9.)

Week 12. Forced convection heat and mass transfer I: confined flows. (Deen chapter 10.)

Week 13. Forced convection heat and mass transfer II: unconfined flows. (Deen chapter 11.)

Week 14. Transport in buoyancy-driven flow. (Deen chapter 12.) Transport in turbulent flow. (Deen chapter 13.)

Week 15. Simultaneous energy and mass transfer *and* multicomponent systems. (Deen chapter 14.) Transport in electrolyte solutions. (Deen chapter 15.)

Advanced Modeling for Catalysis Studies

Instructor: Jeffrey Greeley
Room 2154, Forney Hall
Tel: 41282; email jgreeley@purdue.edu
Office Hours: by appointment.
Classes: Lectures 1:30-2:45, TTh, ARMS 1021.

Course Description: Basic tools needed for theoretical modeling of heterogeneous catalytic systems. Survey of quantum mechanical and statistical mechanical underpinnings of catalysis modeling. Discussion of available methods to predict kinetics of catalytic reaction networks, including details of microkinetic modeling approaches. Practical experience in performing basic DFT calculations, understanding and critiquing catalytic modeling studies in the literature, and developing useful computational models of particular catalytic chemistries from DFT input.

Suggested textbook (not required): *Density Functional Theory: A Practical Introduction*. David S. Sholl and Janice A. Steckel. This textbook has very useful discussions of practical issues associated with DFT calculations, and it is suggested that students either obtain a copy or share with classmates.

Other useful references:
1) *Concepts of Modern Catalysis and Kinetics*. I. Chorkendorff and J. Niemantsverdriet. This is a good overview of kinetics and theory of surface catalysis from a more experimental perspective.
2) *Principles of Adsorption and Reaction on Solid Surfaces.* R. Masel. This text provides more details on the physics of adsorptive processes on metals.
3) *Introduction to Surface Chemistry and Catalysis.* G. A. Somorjai and Y. Li. This is a classic text that provides a broad overview of the field.
4) *Introduction to Quantum Mechanics.* David J. Griffiths. This text provides an accessible yet rigorous introduction to basic quantum mechanical principles from a physicist's perspective.
5) *The ABC of DFT.* K. Burke. This provides a friendly but rigorous introduction to DFT. Downloadable at https://dft.uci.edu/doc/g1.pdf.

Course outline and topics

1) The first part of the semester will focus primarily on the development of the basic theory needed to understand and perform molecular-level modeling of heterogeneous catalysts. Theory lectures will be supplemented by homework assignments and will be interspersed with practical demonstrations of calculations using periodic Density Functional Theory (DFT) codes. Specific topics to be covered include:
    a. Elementary principles of quantum mechanics and DFT: Using very simple one-dimensional systems, the basic philosophy and approach of quantum mechanical calculations will be introduced, and demonstrations of the great simplifications that can be achieved by use of DFT, as opposed to full quantum chemical analyses, will be made.
    b. Thermodynamics of surfaces: Surface energies, surface phase diagrams, and determination of nanoparticle shapes through Wulff constructions.
    c. Microkinetic rate analysis: Molecular basis for, and formulation of, microkinetic models. Analytical solutions and design equations from numerical solutions.
    d. Development of volcano plots: BEP and scaling relationships: Coverage effects and Monte Carlo simulations. Link between microkinetic theories and volcano plots.

   e. Basic theory of modeling of electrochemical reactions at surfaces.

2) The second part of the semester will involve continuing lectures, interspersed with numerous practical demonstrations and opportunities for hands-on experience performing a combination of DFT calculations, kinetic modeling, and statistical modeling. Students will participate in the following projects:
   a. Perform a detailed literature review, and presentation on, a topic of their choice relevant to modeling and theory of heterogeneous catalysts.
   b. Carry out a term project that may involve one or more of the following components: DFT calculations, microkinetic modeling, simple Monte Carlo calculations, analysis of nanoparticle shapes. The term project may be on the same topic as the literature presentation, but this is not required. If there is strong sentiment in the class, then the literature review and term project might be combined into a single assessment.
3) Although I have focused on the above topics when I have previously taught this course, there is some scope to expand and/or modify the selected topics. To this end, I would welcome feedback from the class during the early parts of the semester.

Assessment:
There is one midterm exam, to be taken sometime in mid-to-late March. The midterm will focus on the more theory-related aspects of the course. An individual literature review on a topic of choice related to modeling of heterogeneous catalysis will be presented later in the semester. In addition, a comprehensive term project, covering the results of original catalytic modeling by the students, will be an important focus of the second part of the semester. The term project may be performed individually or in small groups, pending discussions with the university computing facility. Midterm = 30% of grade, literature presentation = 15% of grade, project = 25% of grade. If the literature presentation and term project are merged, the combined assessment will be worth 40% of the total grade.

Homework assignments will be given approximately every two weeks. Homeworks will be worth 30% of the grade, in total. Based on past experience, the homeworks typically require 5-10 hours per assignment to complete (homework frequency will be reduced later in the semester to accommodate work on term projects). Homeworks will be graded primarily on effort; completion of the homeworks, and evidence that students have put forth an appropriate effort, will result in high marks.

Course Evaluation: course evaluation will be available on line and response is strongly encouraged.

Obligatory statement on ethical conduct: students in CHE 697 are pursuing advanced degrees in engineering and the natural sciences and are expected to uphold the Purdue code of ethics, including:

Honesty on homework. Your homework answers must reflect your own independent work and thinking. Discussion about homework problems is allowed and encouraged. However, do not simply copy homework.

Honesty on midterm. You are expected to work by yourself on the midterm exam. No discussion is permitted on the relevant materials. You can only refer to allowed material as specified. All cell phones and mobile devices must be TURNED OFF during the test. Violations will result in, at least, a failing grade on the assessment piece. Serious cases will result in a failing grade for the course and documentation will be sent to the Dean of Students Office.

COURSE ON NUMERICAL METHODS

<u>FINITE ELEMENT ANALYSIS IN CHEMICAL ENGINEERING:</u>
WITH EMPHASIS ON
SOLUTION OF FREE BOUNDARY PROBLEMS IN FLUID MECHANICS, HEAT/MASS TRANSFER, REACTION ENGINEERING, AND SEPARATIONS

CHEMICAL ENGINEERING 697B
SPRING SEMESTER 2023
Time: MWF 4:30-5:20 PM; **Location:** HAMP 2102)

INSTRUCTOR: PROF. OSMAN A. BASARAN
SCHOOL OF CHEMICAL ENGINEERING (OFFICE: FRNY 3060)
765-494-4061 (phone); 765-494-0805 (fax); obasaran@purdue.edu

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<u>Course philosophy and objectives.</u> Over the last several decades, finite element methods have emerged as the numerical method of choice in diverse applications in which the equations that govern the transport of momentum, heat, and species have to be solved and/or free boundaries abound. Some well-known applications of the finite element method to these problems have included free surface flows encountered in coating flows, polymer processing, and drop and bubble dynamics; porous media flows such as ones studied in ground water hydrology and contaminant transport; and solidification and phase change problems such as ones solved in analyses of crystal growth and chemical vapor deposition. This course will emphasize (but not be restricted to) the fundamentals and applications of the finite element method to nonlinear free boundary problems. No prior knowledge of or familiarity with numerical methods will be assumed. Throughout the course, finite difference and analytical methods will be taught side-by-side with finite element methods to enhance the value and applicability of the course to subjects other than those that will be covered during the semester. This course supplements the fine selection of other courses on finite element methods that are offered at Purdue University by focusing on situations in which fluid-fluid and fluid-solid interfaces play a dominant role. The course material is suitable for and should be of interest to students from all engineering disciplines, the sciences (especially physics), and applied mathematics.

<u>Course outline.</u> The course will cover most of the following topics (coverage varies slightly from year to year), beginning with the fundamentals and then quickly moving on to apply the methods to certain problems at the frontiers of research.

Finite elements: one-, two-, and three-dimensional linear and nonlinear, steady and time-dependent problems; basis functions; ordinary and partial differential equations; integral equations; direct and iterative matrix solvers; automatic and adaptive mesh generation, and moving elements.

Stability analysis: turning and bifurcation points.

Applications. Examples from:

- capillary hydrostatics and solutions of the Young-Laplace equation;
- flows governed by the Navier-Stokes and the Euler equations, mixed-interpolation and penalty methods;
- free surface flows and free boundary problems — algebraic and elliptic mesh generation, drop dynamics, film and coating flows, flows with interface rupture, and problems with phase change (e.g. solidification and vaporization);
- flows with heat, mass, and charge transport — surface tension gradient-driven flows, electrohydrodynamics (i.e. coupled solution of the Cauchy momentum and Maxwell's equations), and flows encountered in the processing of electronic materials;
- polymer processing, rheology, and non-Newtonian fluid mechanics;
- separations and reaction engineering.

Other methods: survey of boundary element or boundary integral, finite difference, volume of fluid, level set, boundary collocation, and perturbation methods.

Instructional method. Extensive handouts of lecture notes and supplementary materials, algorithms, and computer programs. Homework (including writing of computer programs), test(s), and project. The latter may be open-ended and lead to publications and/or inclusion in M.S./Ph.D. theses. By the end of the course, participants will be able to read the research literature and use finite elements in their research/work. In past years, a small number of lectures on a hot or specialized topic has also been presented by an expert on that topic. This year, a number of such hot topical areas may once again be covered by several outside experts. These special lectures will be announced during the course of the semester.

Prerequisites. Class participants either should be familiar with or willing to learn during the course of the semester (a) using computers and FORTRAN, C, or some other high-level programming language (MATLAB is also acceptable), (b) vector and tensor analysis at the level of Chapter 6 of Hildebrand's *Advanced Calculus for Applications* and Appendix A of Bird, Stewart, and Lightfoot's *Transport Phenomena* (BSL), and (c) basics of transport phenomena at the level of BSL. A good background in calculus and ordinary and partial differential equations will also be helpful but no previous knowledge of numerical methods will be assumed.

Required and/or supplementary texts.

The following textbook is **required** during Spring Semester 2023:

1. M. S. Gockenbach, *Understanding and Implementing the Finite Element Method*, SIAM (2006).

The following textbook is a **recommended** supplementary book but is **not required** during Spring Semester 2023:

2. W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes*, Cambridge U. Press (2007).

Moreover, the following books are highly recommended as general supplementary texts:

(i) G. Strang and G. J. Fix, *An Analysis of the Finite Element Method*, Prentice-Hall (1973). [The second edition of this classic, which was republished in 2008 by Wellesley-Cambridge Press, has a new part II that focuses on implementation issues.]

(ii) J. N. Reddy and D. K. Gartling, *The Finite Element Method in Heat Transfer and Fluid Dynamics*, CRC Press (1994). [The third edition of this book was published in 2010. I do not recommend this book as a textbook from which one can learn finite elements.]

(iii) L. Lapidus and G. F. Pinder, *Numerical Solution of Partial Differential Equations in Science and Engineering*, Wiley-Interscience (1982). [Just because a book is old does not mean it is not good!]

For most of the material to be presented in the course, there are no appropriate texts. Therefore, lecture notes and handouts will be used primarily to communicate the material to the class participants during the course of the semester. A list of additional supplementary (reference) texts will be given out in class.

Course history. This course has its roots in a one-credit seminar/course taught by the instructor and his colleagues while he was a graduate student in the Department of Chemical Engineering and Materials Science at the University of Minnesota. Since that time, the scope of the course has naturally greatly broadened. In particular, the course being offered is a direct offshoot of a graduate level course which was taught by the instructor biennially over a period of several years at the University of Tennessee and the Oak Ridge National Laboratory. The more recent versions of the course have previously been taught at Purdue University during a number of spring semesters beginning in 1996.