Western Engineering

Department of Chemical & Biochemical Engineering

CBE 4417A – PRINCIPLES AND APPLICATIONS OF HETEROGENEOUS CATALYSIS
COURSE OUTLINE - FALL 2025

Calendar Description
An introduction to the kinetics, mechanisms and chemical fundamentals of heterogeneously catalyzed reactions in the context of modern industrial catalytic processes.

Course Summary
This course is an introduction to the science and engineering of heterogeneous catalysis. The course extends previously learned notions of chemical kinetics and thermodynamic equilibrium to the analysis of surface catalyzed chemical reactions. The concepts of adsorption and desorption together with their thermodynamic and kinetic description are presented. The chemical mechanism of catalysis by surfaces is also explored. The course describes the structure and surface properties of solid catalysts and briefly introduces some of the methods for their characterization, illustrating how the information obtained can be translated into a model for a catalytic active site and a rigorous description of a catalytic reaction mechanism. Important industrial processes including the Fischer-Tropsch synthesis of hydrocarbons, the Haber-Bosch ammonia synthesis, the automotive catalytic converter and hydrotreatment processes will be discussed and used as examples throughout the course.

Prerequisite
CBE3315A/B or GPE3315A/B, CBE2206A/B

Corequisite
None.

Antirequisite
None

Note: It is the **student's responsibility** to ensure that all Prerequisite and Corequisite conditions are met or that special permission to waive these requirements has been granted by the Program. It is also the **student's responsibility** to ensure that they have not taken a course listed as an Antirequisite. The student may be dropped from the course or not given credit for the course towards their degree if they violate the Prerequisite, Corequisite or Antirequisite conditions.

Class Attendance Policy
Class attendance is mandatory and will be monitored. The instructor reserves the right to request debarring from the final examination to those students that miss more than 50% of

lectures in the term.

Course Instructor

J. E. Herrera (TEB 463) Telephone: 519-661-2111 ext: 81262 email: jherrer3@uwo.ca

Undergraduate Coordinator

TEB 477, Telephone: 519-661-2111 ext: 82131 email: cbeugrad@uwo.ca

Reference textbooks:

- *Fundamental Concepts in Heterogenous Catalysis,* J. Norskov, F. Studt, F. Abild-Pedersen, T. Bligaard. Wiley, New Jersey, 2014
- *Spectroscopy in Catalysis: An Introduction*, J. W. Niemantsverdriet (3rd Ed.) Wiley-VHC, Weinheim 2007
- *Concepts of Modern Catalysis and Kinetics* I. Chorkendorff and J.W. Niemantsverdriet (2nd Ed.), Wiley-VHC, Weinheim 2007
- *Catalysis: Concepts and Green Applications*, G. Rothenberg, Wiley-VHC, Weinheim 2008
- *Fundamentals of Chemical Reaction Engineering*, M. Davis and R. Davis, McGraw Hill, New York, 2005

Course content

I. Review of key concepts on Chemical Kinetics and Thermodynamics
- Review of the kinetics vs. thermodynamic control of chemical reactions.
- Case study 1. Kinetic vs. thermodynamic control: The Haber-Bosch ammonia process and the conversion of CO_2 to fuels.
- Overview of Transition State Theory
- Surface potentials and the reaction coordinate. Hammond's Postulate: The link between thermodynamics and chemical kinetics.
- Activation energy changes introduced by a catalytic reaction route.

II. Introduction to heterogeneous catalysis
- General overview of catalytic phenomena: The seven steps of a heterogeneously catalyzed reaction.
- Reaction regimes, external and internal transport effects.
- The Thiele modulus and the effectiveness factor
- Case study 2: The Aromatic complex in the catalytic reforming of naphtha
- Adsorption and Desorption.
- Langmuir-Hinshelwood, Eley-Rideal and Mars-Van Krevelen surface kinetics.
- The Mars and the Weiss-Prater criteria and the impact of transport effects on catalyst performance.
- Case study 3: Engineering an industrial catalyst pellet.

III. Microscopic modeling of heterogeneous catalyzed reactions
- Modeling heterogenous catalyzed reactions using Langmuir-Hinshelwood or Eley-Rideal kinetics
- Modeling surface kinetics: derivation of intrinsic rate laws.
- Case study 4: Surface kinetics modeling on the production of acetaldehyde from ethanol.

IV. Nanoscopic modeling: Surface reactivity and the catalytic active site
- Definition of the catalytic active site and turnover frequencies.
- Case study on the definition of the active site: Hydrotreatment of crude oil
- Chemical description of chemisorption: dissociative and non-dissociative cases.
- Case study 5: The Fischer-Tropsch synthesis of hydrocarbons.
- Case study 6: The catalytic converter and exhaust emissions.
- Volcano plots, descriptors of catalytic activity and the Brønsted-Evans-Polanyi relation

Learning outcomes

Students successfully completing the course will be able to:

- Apply previously learned concepts in chemical kinetics, mass transfer and thermodynamics to the description of heterogeneous catalytic phenomena.
- Provide a quantitative description of surface adsorption and desorption.
- Model surface kinetics and identify reaction limiting steps in heterogeneously catalyzed reactions. *Note: this learning outcome is selected for the assessment of the graduate attribute "Problem Analysis" (PA3, LEVEL: Applied): An ability to use appropriate knowledge and skills to identify, formulate, analyze and solve complex engineering problems in order to reach substantiated conclusions.*
- Recognize external and internal transport limitations in heterogeneously catalyzed reactions. *Note: this learning outcome is selected for the assessment of the graduate attribute "Use of Engineering Tools" (ET2, LEVEL: Applied): An ability to create, select, apply, adapt, and extend appropriate techniques, resources, and modern engineering tools to a range of engineering activities, from simple to complex, with an understanding of the associated limitations.*
- Model external and internal diffusion at steady state in heterogeneously catalyzed processes.
- Deliver the concept of catalytic active site, of structure-activity relationships and recognize the importance of identifying descriptors of catalytic activity.
- Rationalize chemisorption and catalytic active site chemistry using molecular orbital theory.
- Classify different types of catalytic processes in terms chemical considerations.

- Interpret kinetic data and use it to rationalize catalytic phenomena
- Appreciate the current challenges in catalysis and the time evolution of catalytic technology as directed by societal needs.
- Recognize the link between reaction thermodynamics and chemical kinetics.

Graduate Attribute Assessment for Accreditation by the Canadian Engineering Accreditation Board

Graduate Attribute	Indicator	Assessment tool	Assessment Level
Problem Analysis	PA 3 – Demonstrate ability to reach substantiated conclusions.	Assignment 2.	A: Applied
Use of Engineering Tools	ET 2 – Demonstrates ability to apply appropriate engineering tool(s) and resources	Assignment 3.	A: Applied

Course Notes

Some of the course notes (not all) will be available for download from the course website. However, solutions to the problems and some of the materials used for discussions in class will not be posted in the course website. It is expected that notes on these materials will be recorded by the students during the lecture.

Units

SI units will be the primary units used in lectures and examinations.

Evaluation

The final mark will be calculated as follows:

Class Participation	10%
Group assignments (4 in total)	30%
Midterm exam	30%
Final exam	30%

Class participation is not based solely on class attendance, students must actively engage on discussions, and problem-solving during lectures and tutorials. Attendance and participation will be closely monitored and evaluated weekly.

The assignments will be carried in groups of 2 or 3 students.

The midterm exam will take place on Wednesday October 21st at 1:30pm

Examinations will be 2 hours. Exam will be closed book: only handheld non-programmable calculators may be brought to the examinations. Notes, textbooks and other reference materials will not be allowed. **There will be no make-up assignments or exams.** If you are unable to compete an assignment due to medical or compassionate reasons, you must provide the appropriate documentation, and the weighting of the final exam will be adjusted accordingly. Failure to provide the adequate documentation will result in a mark of 0 for the missing course component.

Policy on the use of Mobile Devices

Given that this course covers complex topics requiring focused attention, a policy on electronic devices has been established to ensure a productive and collaborative learning environment for all.

Silent and Stowed: Prior to the beginning of each class, all mobile phones and other electronic devices should be silenced and put away. They are not to be kept on desks or laps, as their presence can be distracting to the instructor and your peers.

Non-Academic Use Prohibited: The use of electronic devices for non-academic purposes—including texting, web browsing, and social media—is not permitted during lecture time. The taking of photos of lecture slides is also prohibited unless explicit permission has been given.

Authorized Use: At specific times, the use of devices for in-class activities such as polls or quizzes may be authorized. Students will be informed when it is appropriate to use their devices for these purposes.

Emergency Situations: In the event that a student is expecting an urgent or emergency call, the instructor should be notified before class. If a call must be taken during class, it is to be done quietly outside the classroom.

Non-compliance with this policy will be documented. Repeated violations may result in a reduction of the course participation grade and may be subject to further disciplinary action in accordance with university academic regulations.

Academic consideration for missing course components

The Faculty of Engineering Policy Framework on Missed Classes, Late Work, and Academic Integrity can be found at:

https://www.eng.uwo.ca/undergraduate/academic-support-and-accommodations/UG-Policy-Framework-Missed-Classes-Late-Work-and-Academic-Integrity.pdf

Please note that BOTH the midterm and final examinations are central to the learning objectives for this course. Accordingly, students seeking academic consideration for this assessment will be required to provide formal supporting documentation. Students who are granted academic consideration for the midterm exam will have the weighting of the final exam adjusted to 60% to account for the missed midterm examination.

For the case of the group assignments, because the submission deadline for these reports already includes flexibility in the form of an automatic 48hr extension, the instructor will deny academic consideration requests supported only by self-attestation for reports which are submitted following the end of the period of flexibility.

Please note that academic consideration requests using formal supporting documentation (medical certificate, etc.) are handled by the Faculty of Engineering Undergraduate Services office.

Repeating All Components of the Course

In accordance with Senate and Faculty Policy, students who have failed an Engineering course (i.e. <50%) must repeat all components of the course. No special permissions will be granted enabling a student to retain laboratory, assignment or test marks from previous years. Previously completed assignments and laboratories cannot be resubmitted for grading by the student in subsequent years.

Use of English

In accordance with Senate and Faculty Policy, students may be penalized up to 10% of the marks on all assignments, tests, and examinations for the improper use of English. Additionally, poorly written work with the exception of the final examination may be returned without grading. If resubmission of the work is permitted, it may be graded with marks deducted for poor English and/or late submission.

Attendance

Attendance to the lectures and tutorials is mandatory and will be monitored. Any student who, in the opinion of the instructor, is absent too frequently from class or tutorial periods will be granted a mark of zero for course participation and will be reported to the Dean (after due warning has been given). On the recommendation of the Department concerned, and with the permission of the Dean, the student will be debarred from taking the final exam in the course.

Marked assignments, projects, quizzes and exams

All marked materials (except for the final examination) will be made available to the students within 10 business days of the examination or laboratory report deadline. Marked exams will be returned during lecture hours. Students are required to pick up and archive their marked materials. It is not the instructor responsibility nor the teaching assistants' to archive or store unclaimed marked exams/laboratory reports.

Cheating

University policy states that cheating is a scholastic offence. The commission of a scholastic offence is attended by academic penalties, which might include expulsion from the program. If you are caught cheating, there will be no second warning (see Scholastic Offence Policy in the Western Academic Calendar).

Plagiarism

Students must write their essays and assignments in their own words. Whenever students take an idea, or a passage from another author, they must acknowledge their debt both by using quotation marks where appropriate and by proper referencing such as footnotes or citations. Plagiarism is a major academic offence (see Scholastic Offence Policy in the Western Academic Calendar).

Sickness and Other Problems

Students should immediately consult with the instructor or Associate Chair (Undergraduate) if they have problems that could affect their performance in the course. The student should seek advice from the Instructor or Associate Chair (Undergraduate) regarding how best to deal with the problem. Failure to notify the Instructor or the Associate Chair (Undergraduate) immediately (or as soon as possible thereafter) will have a negative effect on any appeal. Please contact the course instructor if you require material in an alternate format or if any other arrangements can make this course more accessible to you. You may also wish to contact Services for Students with Disabilities (SSD) at 661-2111 x 82147 for any specific question regarding accommodation.

Accommodation and Accessible Education

The instructor and teaching assistants are not qualified to propose either accommodation strategies nor produce alternative formats for course content aimed at addressing specific accessibility requests. Please contact the Accessible Education office at 661-2111 x 82147 (http://academicsupport.uwo.ca/accessible_education/index.html) for any specific question or request regarding accommodation. The instructor will try to implement accommodation strategies suggested by the Accessible Education office, upon receiving adequate training and resources aimed at addressing the specific student's request.

When a course requirement conflicts with a religious holiday that requires an absence from the University or prohibits certain activities, students should request accommodation for their absence in writing at least two weeks prior to the holiday to the course instructor and/or the Academic Counselling office of their Faculty of Registration. Please consult University's list of recognized religious holidays (updated annually) at:
https://multiculturalcalendar.com/ecal/index.php?s=c-univwo

Notice

Students are responsible for regularly checking their Western email and notices posted on the Brightspace course site.

Consultation

Office hours will be arranged for the students to see the instructor. Other individual consultation during business hours can be arranged by appointment.

Email policy

Students wishing to communicate with the instructor by email should write “CBE4417a question” on the subject line. Email queries linked to the course are checked only twice a day. Students should allow a minimum of 2 business days to get a reply.