Western Engineering

Department of Chemical & Biochemical Engineering

CBE 4417A – PRINCIPLES AND APPLICATIONS OF HETEROGENEOUS CATALYSIS
COURSE OUTLINE - FALL 2026

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, transport phenomena 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.

Contact Hours/Location
3 Lecture hours a week,
1 tutorial hour a week

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 35% of lectures in the term.

Course Instructor

Undergraduate Coordinator

Reference textbooks:

- *Fundamental Concepts in Heterogeneous 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-VCH, Weinheim 2007
- *Concepts of Modern Catalysis and Kinetics* I. Chorkendorff and J.W. Niemantsverdriet (2nd Ed.), Wiley-VCH, Weinheim 2007
- *Fundamentals of Chemical Reaction Engineering*, M. Davis and R. Davis, McGraw Hill, New York, 2005

Course content

I. Kinetic and thermodynamic control in catalytic processes

- Case study 1: Calculating the amount of catalyst required in a packed bed reactor for the isomerization of n-pentane.
- Reversibility and equilibrium limits on conversion. Thermodynamic equilibrium constants in a rate expression.
- Non-elementary rate laws.
- The heterogeneous catalyst as a solid. Physical, mechanical and chemical criteria.
- Transport as a control regime and its impact on heterogeneous catalytic processes.
- The seven steps of a heterogeneously catalyzed reaction.

II. Macroscopic modeling: Transport and reaction in catalyst pellets

- External and internal mass transfer in a catalyst pellet. Reaction regimes and transport effects.
- The Thiele modulus and the effectiveness factor
- Case study 2: The Aromatic complex in the catalytic reforming of naphtha
- The Mears and the Weisz-Prater criteria and the impact of transport effects on catalyst performance.

- Heat transfer effects in a heterogeneously catalyzed reaction, the Arrhenius and the Prater number.
- Case study 3: Engineering an industrial catalyst pellet.

III. Microscopic modeling of heterogeneously catalyzed reactions
- Adsorption and Desorption.
- Langmuir-Hinshelwood and Eley-Rideal surface kinetics.
- Modeling surface kinetics: derivation of intrinsic rate laws.
- The Mars-Van Krevelen mechanism
- 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 5: The definition of the active site in the hydrotreatment of crude oil.
- Chemical description of chemisorption: dissociative and non-dissociative cases.
- Characterization of the catalytic active site: infrared spectroscopy and temperature-programmed desorption.
- Case study 6: The Fischer-Tropsch synthesis of hydrocarbons.
- Case study 7: The catalytic converter and exhaust emissions.
- Descriptors of catalytic activity, the Hammond's postulate and the Brønsted-Evans-Polanyi relationship.
- Volcano plots and the optimum of catalytic activity.

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.
- Explain 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 of 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 3.	A: Applied
Use of Engineering Tools	ET 2 – Demonstrates ability to apply appropriate engineering tool(s) and resources	Assignment 2.	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 (3-4 in total)	30%
Midterm exam	30%
Final exam	30%

EXAMINATION DATES ARE TENTATIVE AND SUBJECT TO CHANGE. Any changes will be communicated in class and via Brightspace.

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 out in groups of 2 or 3 students.

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 complete 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. Illness, injury, or compassionate circumstances that affect attendance or the completion of a course component are handled by the Academic Counselling office in Undergraduate Services, not by the instructor. Students in these circumstances should contact that office directly and as early as possible.

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 misses more than 35% of the lecture or tutorial periods in the term 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's 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).

Accessibility and Academic Accommodation

The instructor and teaching assistants are not qualified to recommend, design, or propose accommodation strategies. Students requiring academic accommodation on the basis of a disability or accessibility need — for example additional time on examinations, alternate formats, or assistive technology — must register with Accessible Education at 661-2111 x 82147 (http://academicsupport.uwo.ca/accessible_education/index.html). That office will communicate approved accommodations to the instructor directly, and will provide the guidance and resources required to implement them. The instructor will implement the accommodations as communicated by Accessible Education. **All questions or requests regarding academic accommodation must be directed to the Accessible Education office, which is the student's first point of contact for these matters — not the instructor.**

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 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.