The University of Western Ontario Faculty of Engineering

DEPARTMENT OF CHEMICAL AND BIOCHEMICAL ENGINEERING

CBE 4427 – AI in Chemical Engineering

Course Outline 2025-2026

In chemical and biochemical engineering, practitioners frequently encounter complex challenges that demand problem-solving and decision-making skills in various areas, including process and product design, fault diagnosis and control, optimization, and process operations and safety. Traditionally, chemical engineers have been adopting modeling concepts and techniques from diverse fields such as applied mathematics and operations research. Over the last three decades, integrating Artificial Intelligence (AI) methods into these approaches has become increasingly prevalent. The necessity for incorporating AI-based techniques into the skillset of well-trained chemical engineers has now been evident. This course seeks to address this crucial need.

Pre-requisites:

Knowledge of statistics, calculus, and linear algebra is required, Python/MATLAB programming skills are strongly recommended. Course requirements: CEB 2291a/b and one course from CS1026a/b and ES1036a/b.

Contact Hours: 3 lecture hours, 1 tutorial hour.

Instructor(s):

Tianlong (Taylor) Liu (TEB 353) tianlong.liu@uwo.ca Undergraduate Assistant: (TEB 477) 519-661-2111 ext: 82131

Course Notes:

Course Notes will be available on the course's OWL site. Students are recommended to bring laptops or other electronic devices that can run either Python or MATLAB to practice in-class activities.

Recommended References:

There is no specific textbook mandatory for this course. Students can read the listed books for their own reference. Several papers from the literature will be made accessible during the course.

- 1. Machine learning: a probabilistic perspective, Kevin P. Murphy, MIT press, 2012.
- 2. Pattern Recognition and Machine Learning, Christopher M. Bishop, Springer, 2006.
- 3. Python for Data Analysis, 3E, 2022. https://wesmckinney.com/book/
- 4. Applied Numerical Methods with MATLAB for Engineers and Scientists, 3/e, Steven C. Chapra, McGraw-Hill Higher Education, 2012.

Units: SI and other units will be used.

Applicable CEAB Attributes:

The table below identifies the attributes that are introduced, taught, and evaluated. The course provides students with a set of artificial intelligent tools and algorithms and teaches students the incorporation of AI-based modeling alongside first-principles models, which can be used to solve complex nonlinear problems in chemical and biochemical engineering. Students are judged as: below expectations, meet expectations and exceed expectations.

Attribute	Classification	Level
Knowledge Base	Taught	Intermediate
Problem Analysis	Taught and evaluated	Intermediate
Investigation	Taught	Intermediate
Design	Taught	Intermediate
Engineering Tools	Taught and evaluated	Intermediate
Individual Work	Taught	Intermediate
Teamwork	Taught	Intermediate
Communication	Taught	Intermediate
Life-Long Learning	Taught and evaluated	Intermediate

Evaluation Methodology of the Applicable CEAB Attributes:

Problem Analysis

Specific Indicators

- The student can identify engineering problems and choose optimum machine learning (ML) algorithms and tools to provide practical solutions.
- The student can successfully apply suitable ML algorithms to model basic chemical and biochemical systems.

Engineering Tools

Specific Indicators

- The student can implement and customize ML algorithms in MATLAB, Python or other platforms.
- The student can import experimental data and analyze the data statistically via various tools.

Life-Long Learning

Specific Indicators

• The student recognizes AI is a powerful tool to solve engineering problems.

• The student is capable to transfer algorithms developed in python or MATLAB to an alternative software package.

Course outline and Learning objectives:

This course is specifically designed for chemical and biochemical engineering students. It aims to impart the knowledge of integrating AI-based modeling with first principle /physical models that are commonly used in the fields of chemical and biochemical engineering, which stem from a comprehensive understanding of physics, chemistry, and biology of products, processes, and systems. To achieve this objective, the course combines traditional numerical modeling and first principle modeling approaches with modern data-driven AI, setting it apart from standard data science courses that typically focus solely on data-driven aspects.

The course will cover topics including chemical engineering modeling approaches, knowledge representation, symbolic reasoning and inference, knowledge-based systems, statistical data analysis, and various ML and physics informed machine learning (PIML) methods. These topics will be explored through chemical engineering case studies in areas such as process monitoring, diagnosis, control, process/product design, scheduling, optimization, and process hazards analysis. A key focus of the course will be on developing hybrid models that merge first-principles knowledge of underlying physics, chemistry, and biochemistry with data-driven techniques, as well as creating causal mechanism-based models. This course will also introduce and incorporate the use of generative AI tools, such as ChatGPT. These tools will be used to enhance the learning experience and provide practical applications in the field of chemical and biochemical engineering.

Evaluation:

The final course mark will be determined as follows:

Assignments 50%

Project 50% (using MATLAB, Python, TensorFlow and/or Keras)

This course has a total of 5 assignments. <u>The lowest assignment grade, including a missed assignment, will be dropped from consideration when calculating your final overall grade for assignments.</u> As such, requests for academic consideration for assignments will be denied.

Note: Late assignments or missed assignments will lead to **a grade of zero** for that element unless an official request for academic consideration/accommodation following the university's policy is submitted and approved. Students must refer to the <u>Policy on Academic Consideration for Medical Illness — Undergraduate Students</u> for details on how to apply for academic consideration/accommodation.

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 in all lectures and tutorials is mandatory. Students are expected to arrive at lectures on time, and to conduct themselves during class in a professional and respectful manner that is not disruptive to others. Any student who, in the opinion of the instructor, is absent too frequently from class or tutorials, will be reported to the Dean (after a 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 writing the project in the course.

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. Scholastic offenses are taken seriously and students are directed to read the appropriate policy, specifically, the definition of what constitutes a Scholastic Offence, at the following Web site: http://www.uwo.ca/univsec/pdf/academic_policies/appeals/scholastic_discipline_undergrad.pdf. All required submissions may be subject to submission for textual similarity review to the commercial plagiarism detection software under license to the University for the detection of plagiarism. All papers submitted for such checking will be included as source documents in the reference database for the purpose of detecting plagiarism of papers subsequently submitted to the system. Use of the service is subject to the licensing agreement, currently between The University of Western Ontario and Turnitin.com (http://www.turnitin.com)

Students are permitted to use generative AI tools like ChatGPT **only if** the specific assignment or project explicitly indicates that such use is allowed. Any unauthorized use of these tools will be considered a violation of academic integrity.

Conduct:

Students are expected to arrive at lectures on time, and to conduct themselves during class in a professional and respectful manner that is not disruptive to others.

Sickness and Other Problems:

Students should immediately consult with the Undergraduate Services if they have any problems that could affect their performance on the course. Where appropriate, the problems should be documented. The student should seek advice from Undergraduate Services regarding how best to

deal with the problem. Failure to notify Undergraduate Services immediately (or as soon as possible thereafter) will have a negative effect on any appeal.

Students who are in emotional/mental distress should refer to Mental Health@Western http://www.uwo.ca/uwocom/mentalhealth/ for a complete list of options about how to obtain help.

Notice:

Students are responsible for regularly checking their email and notices posted on the dedicated OWL site.

Consultation:

Students are encouraged to discuss problems with their teaching assistant and/or instructor in tutorial sessions. Office hours will be arranged for the students to see the instructor and teaching assistants. Other individual consultations can be arranged by appointment with the appropriate instructor.

Accreditation (AU) Breakdown:

Math = 40% Engineering Science = 30% Engineering Design = 30%

Statement on Gender-Based and Sexual Violence:

Western is committed to working to end gender-based and sexual violence on campus and in our community and providing compassionate support to anyone who has gone through these traumatic events. If you have experienced gender-based or sexual violence (either recently or in the past), please connect with a case manager or set up an appointment (support@uwo.ca).