PET E 675 Advanced Thermodynamics and Phase Behavior

Fall 2025

Instructor:
Dr. Zhehui Jin
Office: DICE 6-304
Phone: 213-822-2811
Email: zhehui2@ualberta.ca

Course Webpage: *eClass*

Prerequisites: PET E 373 or consent of instructor

Course Synchronized Lecture Time: 2:00 - 4:50 pm Edmonton Time F

Course Objectives:

This course introduces molecular-level modeling of adsorption, diffusion, and transport phenomena in porous media, with applications to shale/tight formations and energy storage. Students will learn fundamental statistical thermodynamics, Monte Carlo and molecular dynamics simulation techniques, and practical use of Towhee and LAMMPS software. The course combines lectures, partial labs, and full lab sessions, culminating in a final project on multicomponent adsorption in different pore types, sizes, and temperatures.

Suggested References:

- Allen, M. P., & Tildesley, D. J. Computer Simulation of Liquids, 2nd Edition, Oxford University Press, 2017
- Frenkel, D., & Smit, B. Understanding Molecular Simulation, 2nd Edition, Academic Press, 2002
- Rouquerol, F., Rouquerol, J., & Sing, K. Adsorption by Powders and Porous Solids, 2nd Edition, Academic Press, 2013
- Emami, F., et al., J. Phys. Chem. B, 2014, 118, 11105–11117
- Additional journal articles will be assigned as needed

Learning Outcome:

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

1. Apply statistical thermodynamics to adsorption phenomena.
2. Model adsorption and transport in porous media using Monte Carlo and molecular dynamics simulations.

3. Characterize pores from adsorption data (NLDFT approach).

4. Simulate convection and diffusion in bulk and confined systems.

5. Conduct independent computational projects on multicomponent adsorption and diffusion, and analyze results.

Course Evaluation and Grading: The course evaluation comprises of four components as indicated by the following mark distribution.

Tasks	Weight, %	Date/Frequency	Place
Class Participation	10	Every Class	In Class
Partial Lab Exercise	20	5 Times	In Class
Full Lab Reports	30	3 Times	Online
Final Project	40	1 Time	Online

The final academic performance of students in this course will be evaluated based on the following grade guideline. All grades remain unofficial until approved by the Department and/or Faculty offering the course.

Descriptor	Letter Grade	Grade Point Value
	A+	4.0
Excellent	A	4.0
	A-	3.7
	B+	3.3
Good	B	3.0
	B-	2.7
Satisfactory	C+	2.3
	C	2.0
	C-	1.7
Failure	D+	1.3
	D	1.0
	F	0.0

Weekly Schedule (Tentative):

Week 1 (Sep 5): Introduction & Shale/Tight Formation Characteristics (Discussion)

Week 2 (Sep 12): Basic Statistical Thermodynamics; Partition Function; Ensemble Averages

- Partial Lab 1: Setup Compute Canada accounts, install Towhee and LAMMPS

Week 3 (Sep 19): Adsorption Thermodynamics; Single-Component Isotherms (Langmuir/BET)

- Partial Lab 2: Running basic Towhee scripts; generating initial adsorption data

Week 4 (Sep 26): Monte Carlo Simulation Overview; Towhee Setup

- Partial Lab 3: Adsorption simulations; extracting density profiles

Week 5 (Oct 3): Multicomponent Adsorption Principles; Competitive Effects

Week 6 (Oct 10): Full Lab 1 – Single-Component Adsorption

Week 7 (Oct 17): Pore Characterization Session: Connect adsorption isotherms to NLDFT

Week 8 (Oct 24): Convection Concepts and Slip Length

- Full Lab 1: Help Sessions

Week 9 (Oct 31): Single-Component Diffusion Concepts

- Partial Lab 4: LAMMPS setup and basic convection runs

Week 10 (Nov 7): Full Lab 2 – Convection & Parallel Computing in LAMMPS

Week 11 (Nov 14): Reading Week – No class

Week 12 (Nov 21): Full Lab 3 – Single-component diffusion in bulk using LAMMPS

Week 13 (Nov 28): Applications: Hydrocarbon Recovery, CO_2 Storage, Energy-Related Porous Systems

- Final Project Setup & Discussion: Multicomponent adsorption in different rocks, pore sizes, and temperatures; optional diffusion integration

Week 14 (Dec 5): Optional Help / Project Preparation Session

Lab Sessions Overview:

Partial Labs:

1. Setting up accounts, installing Towhee & LAMMPS
2. Running Towhee scripts, generating initial adsorption data
3. Extracting density profiles, analyzing adsorption
4. LAMMPS setup, preliminary convection runs
5. LAMMPS setup, bulk diffusion runs

Full Labs:

1. Single-Component Adsorption (Week 6) – Towhee
2. Convection & Parallel Computing (Week 10) – LAMMPS
3. Single-Component Diffusion in Nanopores (Week 12) – LAMMPS

Final Project:

- Multicomponent adsorption in different rocks, temperatures, and pore sizes – Towhee

Final Project Deliverables:

- Written report (methodology, results, analysis, discussion)

- Oral presentation
- Visualizations: adsorption isotherms, density profiles, comparative plots across conditions

Class Participation:

- Attendance, engagement in discussions, questions during labs and lectures

Format of Partial Lab Exercise: The partial lab exercise is conducted within the class. The students are expected to conduct the tasks laid out by the instructor.

Format of Full Lab Report: The full lab report is conducted after the class. The students are expected to learn the tasks and skills needed within the class.

Format of Final Project: The final project includes two elements: project report and presentation. A list of potential topics proposed by the instructor will be announced in the class and posted in Eclass. Every two students will form a team to work on the proposed topic. Each team can also propose a topic, but need to discuss it with the instructor before finalizing.

Academic Integrity: "The University of Alberta is committed to the highest standards of academic integrity and honesty. Students are expected to be familiar with these standards regarding academic honesty and to uphold the policies of the University in this respect. Students are particularly urged to familiarize themselves with the provisions of the Code of Student Behavior (online at www.governance.ualberta.ca) and avoid any behavior which could potentially result in suspicions of cheating, plagiarism, misrepresentation of facts and/or participation in an offence. Academic dishonesty is a serious offence and can result in suspension or expulsion from the University."

Student with Disabilities: Students who require accommodation in this course due to a disability are advised to discuss their needs with Specialized Support & Disability Services (2-800 Students' Union Building).

Academic Support Center: Students who require additional help in developing strategies for better time management, study skills or exam skills should contact the Student Success Centre (2-300 Students' Union Building).

Disclaimer: "Policy about course outlines can be found in §23.4(2) of the University Calendar". Dr. Jin reserves the right to change session topics throughout the semester. Any typographical errors in this Course Syllabus are subject to change and will be announced in class.