CHEMENG 777: Dynamics of Polymers and Complex Fluids

Course Outline – Winter 2026

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INSTRUCTOR

Li Xi

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Office Hours : by appointment

CLASS SCHEDULE

When	Where
Tuesdays 10:30 – 11:20 am Thursdays 10:30 – 12:20 am	Per university policy, class locations are not listed in the course outline, but will be communicated via MS Teams.

TEXTBOOKS AND REFERENCES

Required

- M. Rubinstein and R. H. Colby, *Polymer Physics*, Oxford, 2003 (ISBN: 978-0198520597)

Recommended

- M. Doi and S. F. Edwards, *The Theory of Polymer Dynamics*, Oxford, 1986 (ISBN: 978-0198520337)
- M. D. Graham, *Microhydrodynamics, Brownian Motion, and Complex Fluids*, Cambridge, 2018 (ISBN: 978-1107695931)

Additional References

- R. B. Bird, C. F. Curtiss, R. C. Armstrong, and O. Hassager, *Dynamics of Polymeric Liquids: Vol 2 Kinetic Theory*, 2nd edn., Wiley, 1987 (ISBN: 978-0471802440).
- R. B. Bird, W. E. Stewart, and E. N. Lightfoot, *Transport Phenomena*, 2nd edn. (revised), Wiley, 2006 (ISBN: 978-0470115398).
- W. M. Dean, *Analysis of Transport Phenomena*, Oxford, 1st edn., 1998 (ISBN: 978-0195084948) or 2nd edn., 2012 (ISBN: 978-0199740284).
- M. Doi, *Introduction to Polymer Physics*, Oxford, 1996 (ISBN: 978-0198517894).
- J. M. Dealy, D. J. Read, and R. G. Larson, *Structure and Rheology of Molten Polymers: From Structure to Flow Behavior and Back Again*, revised edn., Hanser, 2018 (ISBN: 978-1569906118); also see the first edition, 2006 (ISBN: 978-3446217713).
- T. C. B. McLeish, "Tube theory of entangled polymer dynamics", *Advances in Physics*, 51, 1379–1527, 2002 (DOI: 10.1080/00018730210153216).
- L. Xi, "Molecular simulation for predicting the rheological properties of polymer melts", *Molecular Simulation*, 45, 1242–1264, 2018 (DOI: 10.1080/08927022.2019.1605600).

*Future revisions of this document will always supersede earlier versions.

The first half of the course (modules 1 and 2) is built on several chapters in Rubinstein & Colby. The second half (modules 3 and 4) is built, for the most part, on contents from Doi & Edwards and Graham, with some contents drawn from "additional references".

COURSE CONTENTS

The course provides an overview of relevant concepts and theories for describing the molecular motion of polymer chains and how the dynamics at molecular scales is related to the materials' response to deformation and flow. Although the course focuses on polymers as its main subject, many of the theories and tools can be extended to more general complex fluids systems.

The course is composed of four modules. Module 1 gives a general introduction to polymer chain conformation and the free energy of conformation changes. Module 2 gives a brief introduction to macroscopic material functions for the deformation and flow of polymer materials and simple conceptual models for those properties. Module 3 lays out the general theoretical framework for describing the dynamics of complex fluids in terms of connecting the microscopic material structure with macroscopic behaviors. Module 4 covers common models of chain dynamics, from which viscoelastic properties of polymer materials can be predicted, of unentangled and entangled polymers. The specific breakdown of the contents is listed as follows*.

1. Polymer Chain Conformation
   (a) Ideal chains
   freely-jointed chain; freely-rotating chain; hindered rotation model; rotational isomeric state; worm-like chain; chain conformation statistics; random walk model; free energy of chain deformation
   (b) Real chains
   excluded volume and intermolecular interactions; solvent conditions; conformation and free energy of real chains
   (c) Other basic terminology
   Pervaded volume and overlap parameter; dilute/semi-dilute solutions
2. Elasticity and Viscoelasticity
   (a) Elasticity and polymer networks
   affine network model; phantom network model; shear and tensile stresses; entangled networks; tube model – basic concepts
   (b) Introduction to linear viscoelasticity
   viscoelasticity and Maxwell model; step strain and relaxation modulus; Boltzmann superposition principle; steady shear; oscillatory shear and dynamical moduli; creep and creep recovery
3. Kinetic Theory – Diffusion and Hydrodynamics
   (a) Single-particle dynamics
   diffusion and Fick's law; vector and tensor algebra; Brownian motion; equation of motion – Langevin equation; fluctuation-dissipation theorem (basic introduction); configuration-space description – Smoluchowski/Fokker-Planck/generalized diffusion equation
   (b) Multi-particle dynamics

microhydrodynamics; hydrodynamic interactions; multi-particle Langevin and Smoluchowski equations; Gaussian chain; dynamics of bead-spring chains

(c) Hydrodynamics of polymer fluids
stress tensor and its kinetic theory; stress tensor of Brownian particles, elastic dumbbells, and bead-spring chains; constitutive equations (Oldroyd-B and FENE-P)

4. Relaxation Dynamics
   (a) Rouse model for unentangled chains
   Rouse model and its equation of motion; normal coordinates (Rouse modes); relaxation of Rouse modes; hydrodynamic interactions and Zimm model; stress tensor and relaxation modulus from the Rouse modes
   (b) Tube model for entangled chains
   entanglement and tube model; reptation dynamics; tube survival probability and relaxation modulus

*The contents are subject to change during the offering at the discretion of the instructor.

ASSESSMENT* †

- Assignments (30%)
- Exams (70%): 12%+12%+12%+34%‡.

*Adjustment/re-curving of the term grade may be applied at the discretion of the instructor.
†The final letter grade will be assigned using the Registrar's recommended procedure.
‡Exams will be oral and held after every module. The last/final exam will be cumulative and cover the entire course contents.

COMMUNICATION

McMaster E-mail Account The "@mcmaster.ca" E-mail accounts will be used for course-related correspondence. Students are expected to check their E-mail accounts regularly.

Microsoft Teams (https://teams.microsoft.com/; also referred to as "MS Teams" or just "Teams") will be used for class-related communications, including online meetings and direct messages. Course materials and important information will also be distributed/communicated using MS Teams. Students are expected to log in regularly to their Teams accounts associated with their MacIDs and be able to receive messages there. Students are also required to join the class's Team* and check for course updates regularly.

*Contact the instructor if you are not in the class Team.

APPROVED ADVISORY STATEMENTS

The following statements are required per McMaster's Undergraduate Course Management Policies.

Academic Integrity

You are expected to exhibit honesty and use ethical behaviour in all aspects of the learning process. Academic credentials you earn are rooted in principles of honesty and academic integrity. **It is your responsibility to understand what constitutes academic dishonesty.**

Academic dishonesty is to knowingly act or fail to act in a way that results or could result in unearned academic credit or advantage. This behaviour can result in serious consequences, e.g. the grade of zero on an assignment, loss of credit with a notation on the transcript (notation reads: "Grade of F assigned for academic dishonesty"), and/or suspension or expulsion from the university. For information on the various types of academic dishonesty please refer to the Academic Integrity Policy, located at https://secretariat.mcmaster.ca/university-policies-proceduresguidelines/.

The following illustrates only three forms of academic dishonesty:

1. plagiarism, e.g. the submission of work that is not one's own or for which other credit has been obtained.
2. improper collaboration in group work.
3. copying or using unauthorized aids in tests and examinations.

Authenticity/Plagiarism Detection

Some courses may use a web-based service (Turnitin.com) to reveal authenticity and ownership of student submitted work. For courses using such software, students will be expected to submit their work electronically either directly to Turnitin.com or via an online learning platform (e.g. A2L, etc.) using plagiarism detection (a service supported by Turnitin.com so it can be checked for academic dishonesty.

Students who do not wish their work to be submitted through the plagiarism detection software must inform the Instructor before the assignment is due. No penalty will be assigned to a student who does not submit work to the plagiarism detection software. **All submitted work is subject to normal verification that standards of academic integrity have been upheld** (e.g., on-line search, other software, etc.). For more details about McMaster's use of Turnitin.com please go to www.mcmaster.ca/academicintegrity.

Courses with an On-Line Element

Some courses may use on-line elements (e.g. e-mail, Avenue to Learn (A2L), LearnLink, web pages, capa, Moodle, ThinkingCap, etc.). Students should be aware that, when they access the electronic components of a course using these elements, private information such as first and last names, user names for the McMaster e-mail accounts, and program affiliation may become apparent to all other students in the same course. The available information is dependent on the technology used. Continuation in a course that uses on-line elements will be deemed consent to this disclosure. If you have any questions or concerns about such disclosure please discuss this with the course instructor.

Online Proctoring

Some courses may use online proctoring software for tests and exams. This software may require students to turn on their video camera, present identification, monitor and record their computer activities, and/or lock/restrict their browser or other applications/software during tests or exams. This software may be required to be installed before the test/exam begins.

Conduct Expectations

As a McMaster student, you have the right to experience, and the responsibility to demonstrate, respectful and dignified interactions within all of our living, learning and working communities. These expectations are described in the Code of Student Rights & Responsibilities (the "Code"). All students share the responsibility of maintaining a positive environment for the academic and personal growth of all McMaster community members, **whether in person or online**.

It is essential that students be mindful of their interactions online, as the Code remains in effect in virtual learning environments. The Code applies to any interactions that adversely affect, disrupt, or interfere with reasonable participation in University activities. Student disruptions or behaviours

that interfere with university functions on online platforms (e.g. use of Avenue 2 Learn, WebEx or Zoom for delivery), will be taken very seriously and will be investigated. Outcomes may include restriction or removal of the involved students' access to these platforms.

Academic Accommodation of Students with Disabilities

Students with disabilities who require academic accommodation must contact Student Accessibility Services (SAS) at 905-525-9140 ext. 28652 or sas@mcmaster.ca to make arrangements with a Program Coordinator. For further information, consult McMaster University's Academic Accommodation of Students with Disabilities policy.

Requests for Relief for Missed Academic Term Work

In the event of an absence for medical or other reasons, students should review and follow the Policy on Requests for Relief for Missed Academic Term Work.

Academic Accommodation for Religious, Indigenous or Spiritual Observances (RISO)

Students requiring academic accommodation based on religious, indigenous or spiritual observances should follow the procedures set out in the RISO policy. Students should submit their request to their Faculty Office ***normally within 10 working days*** of the beginning of term in which they anticipate a need for accommodation or to the Registrar's Office prior to their examinations. Students should also contact their instructors as soon as possible to make alternative arrangements for classes, assignments, and tests.

Copyright and Recording

Students are advised that lectures, demonstrations, performances, and any other course material provided by an instructor include copyright protected works. The Copyright Act and copyright law protect every original literary, dramatic, musical and artistic work, **including lectures** by University instructors.

The recording of lectures, tutorials, or other methods of instruction may occur during a course. Recording may be done by either the instructor for the purpose of authorized distribution, or by a student for the purpose of personal study. Students should be aware that their voice and/or image may be recorded by others during the class. Please speak with the instructor if this is a concern for you.

Extreme Circumstances

The University reserves the right to change the dates and deadlines for any or all courses in extreme circumstances (e.g., severe weather, labour disruptions, etc.). Changes will be communicated through regular McMaster communication channels, such as McMaster Daily News, A2L and/or McMaster email.