

## CHMD59F/CHM1425H/EES1121H

### Modeling the Fate of Organic Chemicals in the Environment

This course will give an introduction to quantitative approaches to describing the behaviour of organic chemicals in the environment. Building upon a quantitative treatment of equilibrium partitioning and kinetically controlled transfer processes of organic compounds between gaseous, liquid and solid phases of environmental significance, it will be shown how to build, use, and evaluate simulation models of organic chemical fate in the environment. The course will provide hands-on experience with a variety of such models.

**Instructor:** F. Wania  
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**Format:** 2-hour lecture, followed by 1-hour tutorials

The lecture and some of the tutorials will be delivered in-person in the class room. They will be recorded and the recordings made available to those who cannot attend in-person by being embedded on Quercus. Student presentations will be delivered through Bb Collaborate during the time slot of the Tutorial, unless a student would prefer to give the presentation in-person.

**Time:** Wednesday, 9:00 to 12:00

**Location:** SY110, UTSC Campus

**Office Hours:** On-line, by appointment only (write e-mail to instructor or TA for scheduling)

**Grading:**

	CHM1425H EES1121H	CHMD59F
2 Take-home assignments	20 %	30 %
Paper summary presentations	10 %	10 %
1 Term project/paper	30 %	30 %
1 Project presentation	10 %	
1 Final take-home exam	30 %	30 %

For those taking the course at the graduate level:

- the expectation with respect to the term project/paper are higher
- a short oral presentation on the term paper/project is expected
- the final exam will include more challenging questions

Evaluation will be carried out in accordance with the Graduate Grading and Evaluation Practices Policy (and how that policy is interpreted and applied in this Dept.)

<https://governingcouncil.utoronto.ca/secretariat/policies/grading-practices-policy-university-assessment-and-january-1-2020>

**Prerequisites:** An introductory course in each of organic, physical and environmental chemistry.

**Textbook:** Not any one text book includes all of the material covered in this course. Reading assignments (e.g. textbook chapters, scientific publications) will be given during each lecture. Useful for reference will be the following books:

Mackay, D. *Multimedia Environmental Models. The Fugacity Approach*. Lewis Publ. Chelsea, MI

Schwarzenbach, R., Gschwend, P., Imboden. *Environmental Organic Chemistry*. J. Wiley & Sons, NY

These books will be available upon request.

## Course Outline

#	Date	Topic (tentative)
1	Sept. 9	Introduction: Motivation and Mass Balance, System Definition
2	Sept. 16	Segmentation/Compartmentalization
3	Sept. 23	Expressing Equilibrium Phase Distribution: Distribution Coefficients and Linear Free Energy Relationships
4	Sept. 30	Expressing Equilibrium Phase Distribution: Measurement, Estimation and Selection of Phase Partitioning Equilibria
5	Oct. 7	Expressing Equilibrium Phase Distribution: Equilibrium Models and the Chemical Partitioning Space
	Oct. 14	UTSC undergraduate reading week
6	Oct. 21	Expressing Kinetic Phenomena: Transformation and Advective Transport
7	Oct. 28	Expressing Kinetic Phenomena: Diffusive Transport Processes and level III Models
8	Nov. 4	Expressing Kinetic Phenomena: Measurement and estimation of mass transfer coefficients and rate constants
9	Nov. 11	Modelling Bioaccumulation and Food Chain Transfer of Contaminants
10	Nov. 18	Examples of Model Application
11	Nov. 25	Examples of Model Application
12	Dec. 2	Student presentations on term project by those taking the course at the graduate level
	Dec. 2	Due date for term papers for those taking the course at the undergraduate level
	Dec. 9	Due date for term papers for those taking the course at the graduate level

### LATE WORK

For every day that an assignment or term paper is handed in late, I will deduct 10 % of the mark on that assignment/report.

### PLAGIARISM

University of Toronto code of Behaviour on Academic Matters states that "it shall be an offense for a student knowingly: to represent as one's own any idea or expression of an idea or work of another in any academic examination or term test or in connection with any other form of academic work, i.e., to commit plagiarism."

For accepted methods of standard documentation formats, including electronic citation of internet sources please see the UofT writing website at: <http://www.writing.utoronto.ca/advice/using-sources/documentation>

The full Code of Behaviour regulations for graduate students could be found from consulting <http://www.sgs.utoronto.ca/facultyandstaff/Pages/Academic-Integrity.aspx>

### EMERGENCY PLANNING

Students are advised to consult the university's preparedness site (<http://www.preparedness.utoronto.ca>) for information and regular updates regarding procedures relating to emergency planning.

### ACCESSIBILITY NEEDS

The University of Toronto is committed to accessibility. If you require accommodations for a disability, or have any accessibility concerns about the course, the classroom or course materials, please contact The UTSC Accessibility Services as soon as possible: <http://www.utsc.utoronto.ca/~ability/>

We also suggest you also refer to the following University of Toronto Scarborough Library link: <http://utsc.library.utoronto.ca/services-persons-disabilities>