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
Office SY-364 (University of Toronto Scarborough)
Tel. 416-287-7225
E-mail: frank.wania@utoronto.ca

Format: 2 hours lecture, followed by 1 hour tutorials

Time: Wednesday, 9:00 to 12:00

Location: SW221, UTSC Campus

Office Hours: Wednesday, 13:00-15:00, or by appointment

Grading:

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

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 in SY-364.

Course Outline

#	Date	Topic (tentative)
1	Sept. 15	Introduction: Motivation and Mass Balance System Definition
2	Sept. 22	Segmentation/Compartmentalisation
3	Sept. 29	Expressing Equilibrium Phase Distribution: Distribution Coefficients and Linear Free Energy Relationships
4	Oct. 6	Expressing Equilibrium Phase Distribution: Measurement, Estimation and Selection of Phase Partitioning Equilibria
5	Oct. 13	Expressing Equilibrium Phase Distribution: Equilibrium Models and the Chemical Partitioning Space
6	Oct. 20	Expressing Kinetic Phenomena: Transformation and Advective Transport
7	Oct. 27	Expressing Kinetic Phenomena: Diffusive Transport Processes
8	Nov. 3	Application of Simple Steady-State Models: Assessment of Persistence and Long Range Transport Potential, Sensitivity and Uncertainty Analysis
9	Nov. 10	Application of Non-Steady-State Models: Understanding Time Trends
10	Nov. 17	Modelling Bioaccumulation and Food Chain Transfer of Contaminants
11	Nov. 24	Modelling Global Contaminant Fate and Transport
12	Dec. 8	Student presentations on term project by those taking the course at the graduate level
	Dec. 15	Due date for term projects/papers

Lectures on Sept. 22, 29 and Nov. 10 will be given by Dr. Torsten Meyer