**CEE 490/690.03 MODELING ENVIRONMENTAL, CHEMICAL, BIOLOGICAL AND ENERGY PROCESSES**
**FALL 2019**

**INSTRUCTOR: Marc Deshusses**, 127C Hudson Hall, marc.deshusses@duke.edu
**TA and TA office hours:** to be announced
**CLASS: Mondays and Wednesdays 10:05-11:20 am Hudson 218**
A majority of the class segments will consist of a mix of lecture and modeling exercises in class with a computer (unless you hear otherwise, bring your laptop)

**OFFICE HOURS:** office hours tbd, also open door policy or meeting on appointment

**TEXT(S)**
No text is required, I will distribute handouts. Do not buy any of the books listed below, unless you have a special interest in owning the book. The first 3 are most relevant, the library has a few of them.

**Books relevant to the course:**
Biological Reaction Engineering: Dynamic Modelling Fundamentals with Simulation Examples (2nd Ed.). I.J. Dunn, E. Heinzle, J. Ingham, J.E. Prenosil. Wiley; New York, 2003.

Chemical Engineering Dynamics: An Introduction to Modelling and Computer Simulation (3rd Ed.). J. Ingham, I.J. Dunn, J.E. Prenosil, J.B. Snape,. Wiley; New York, 2007.

Dynamics of Environmental Bioprocesses: Modelling and Simulation. J.B. Snape, I.J. Dunn, J. Ingham, J.E. Prenosil. Wiley-VCH; New York, 1995. (now a bit dated, but very similar in spirit to the other two books)

Very relevant to the course are modeling papers published in peer reviewed journals such as Biotechnol. Bioeng., Bioproc. Eng., J. Environ. Eng. ASCE. See also COMSOL Newsletter for relatively accessible papers on computational fluid dynamics and multiphysics modeling.

**OBJECTIVES OF THE COURSE**
After attending this course, students will:
1. Recognize that many approaches exist to modeling and simulation, and be able to define the possibilities and limits of modeling
2. Be able to create and troubleshoot their own models
3. Be able to translate key biochemical, chemical, environmental and energy processes into functional models and explore their sensitivity to key parameters
4. Have formulated models relevant to their own research or interest
5. Be capable of utilizing basic function of a computational fluid dynamics (CFD) and multiphysics modeling software (COMSOL), and to apply basic experimental design (factorial design)
6. Have been exposed to research other than their own

**GRADING CEE 690**
Presentations, model simulation exercises, homework, participation: 30%
2 Quizzes (10% each) dates to be announced
Term project: 50% (final report due around final exams week, see separate handout)
(there is no mid-term or final exam)

**A FEW RULES**
-Since there will be only a few homework assignments, it is very important to turn all of them in
-Late homework is not graded; homework is due in class or by email before class starts
-Solutions are posted on Sakai
-Duke usual academic integrity rules apply
-Notify me if you will miss class

**TENTATIVE SYLLABUS (WILL BE ADJUSTED BASED ON YOUR INPUT)**

1. Introduction, Model Classification
2. Model Development
   - 2.1 Basic model development procedure
   - 2.2 Mass and energy balancing
   - 2.3 Algorithms for numerical integration
   - 2.4 Determination of model parameters
   - 2.5 Introduction to Berkeley Madonna software
3. Examples and Applications (see below)
4. Introduction to Computational Fluid Dynamics (CFD) and Multiphysics Modeling using COMSOL
   - 4.1 Introduction to the software
   - 4.2 In class exercise, geometry and system setup
5. Selected topics (to be determined)

## 6. Examples and applications

Below are exercises we may conduct together in class. They are usually preceded by a recap of the corresponding theory (or assigned reading) leading to the model equations. Some models are provided "ready to run", some are partially written and students have to complete them, other are developed from scratch by the students. Many of the models and exercises are "open-ended" and can be expanded to incorporate complex non-linear phenomena.

(tentative list, topics will be adjusted based on students interests)

- 3.0 Integration algorithms
- 3.1 Continuously stirred tank reactors (CSTRs) with 1$^{st}$ and 2$^{nd}$ order reactions, autocatalytic reaction, CSTRs in series
- 3.2 Plug flow reactor (PFR) with non-linear kinetics, steady-state and dynamic model, axial dispersion, parametric sensitivity, array notation, comparison with series of CSTRs
- 3.3 Diffusion and reaction (steady-state and dynamic, integration within a larger system)
- 3.4 Incorporation of, and fitting to experimental data (one and multi-parameter fitting)
- 3.7 Complex reaction (sequential and parallel reactions)
- 3.8 Fate of pesticide in a simplified aquatic ecosystem (2 compound, 3 compartments), and/or nitrogen cycle in a reservoir, and/or Predator-prey dynamics
- 4. Examples and exercises for COMSOL will be announced

## 7. Presentations

Students will be asked to make 2-3 presentations on their modeling assignments, and once on a modeling paper they selected. The objective is to engage in constructive discussions on the topic, discuss challenges and solutions, and practice presentation skills.

## 8. Quizzes

There will be two quizzes of about 30-40 min. Dates, exact format and content will be discussed in class.

## 9. Term project

Each student will be asked to develop his/her own model relevant to his/her interest. Instructor and TA will hold consultation hours to help with model development and debugging. Students will turn in one interim progress report, a final term paper and make a presentation at the end of the semester. The term project model does not need to be very complex, but it should be original. Students should have demonstrated a good understanding of their subject topic and conducted an in-depth analysis of their model. A separate handout will be distributed with more detailed instructions.