Course MATHEMATICAL MODELING

Basic Information

This is a course, which contributes to MSc award in Petroleum Chemistry and Refining

Title of the Academic Program	Master's Degree Programs in English "Mathematical Modeling"
Course period	From October 8th 2018 till January 27th 2019, 2 semester (15 weeks)
Study credits	5 ECTS credits
Duration	180 hours
Language of instruction	English
Academic requirements	– BSc degree in Chemistry, Physics, Mathematics, Engineering, Environmental Sciences or equivalent (transcript of records), – good command of English (certificate or other official document)

Course Description

This course serves as an introduction to mathematical modeling and applied mathematics, more generally. The main objective will be to learn how to take a phenomena arising in physics, chemistry, biology, even the social sciences, then study it (intelligently) using mathematics. This can be a very tricky endeavor: it necessitates both a sound understanding of the field where the problem originated, and a capacity for sometimes quite sophisticated mathematical analysis.

It also typically requires using numerical analysis, that is, using a computer to solve problems that are not tractable by hand. This means that as part of the course you will be asked to use some programs (particularly developed by me).

The planned topics to be covered are:

- Introduction to the Science of Mathematical Modeling;
- Microscopic Scale Models and Ordinary Differential Equations;
- Macroscopic Scale Models and Partial Differential Equations;
- Numerical Methods.

Depending on student interest, and the general flow of the class, we may add items. Please let me know if there is something in particular that you'd like to see covered.

Special Features of the Course

1. Practical aspects of mathematical modeling are tightly integrated in the teaching on the course.

In addition to conventional lectures the course offers a range of other learning opportunities in which students actively participate. Moreover, students will be involved in online tests.

2. The course includes description of total process of modeling staring with learning physical phenomena and ending with predicting the behavior of the phenomena using numerical methods.

3. The educational process is supported with programs which allow to compute solution of differential equations systems. The programs are developed by me within my scientific research.

Course Aim

The overall goal of this course is **to enable students to analyze mathematical models of real-world systems, choose numerical methods to calculate solutions, estimate its behavior and make predictions about behavior of these systems**. Variety of modeling techniques will be discussed with examples taken from physics, biology, chemistry and other fields. The focus of the course will be on seeking the connections between mathematics and physical systems, studying and applying various modeling techniques to creating mathematical description of these systems, and using this analysis to make predictions about the system's behavior.

Course Objectives

- to gather and convert information of a physical phenomena into a mathematical framework;
- to analyze a model and to apply an appropriate method to calculate a solution in order to predict the behavior of the system;
- to interpret results of modeling (what do all those numbers and variables and equations and diagrams and graphs and charts actually mean);
- to communicate the entire process (abstraction, hypothesis, analysis, conclusion) to your intended audience (which may know less, the same amount of, or more mathematics than you do)

Learning Outcomes of the Course

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

- to handle freely the concepts using in mathematical modeling;

- to analyze a simple physical phenomena in order to create a mathematical model;
- to apply numerical methods to solve systems of ordinary differential equations;
- to interpret numerical results given by program in order to predict the behavior of the system;
- to understand the mechanism of mathematical modeling in chemical engineering.

Course Outline

Week	Lectures	Practice session / Assignments	Hours[1]
Introduction to the Science of Mathematical Modeling			
1-3	- An Introduction to Modeling; - Modeling Scales And Representation; - Classification of Models.		1 1 1
		Test your knowledge: basic definitions; Test your knowledge: modeling scales; Test your knowledge: classification; Assignment "Mathematical Modeling Basics".	2 2 2 4
Microscopic Scale Models and Ordinary Differential Equations			
4-7	- Derivation And Classification Mathematical Models; - Solution Schemes And Time Derivation; - Stability Methods.		2 2 1
		Test your knowledge: derivation of models; Test your knowledge: solution schemes; Test your knowledge: stability methods; Assignment "Mathematical Modeling Basics"; Assignment "Solution Methods and Theoretical Considerations".	2 2 2 4 4
Macroscopic Scale Models and Partial Differential Equations			
8-9	- Modeling Methods And Applications; - Classification of Models And		1 1

[1] Hours designed for Classroom sessions, Web-sessions, Home Assignments etc.

	Equations.	Test your knowledge: modeling methods; Test your knowledge: classification of models; Assignment "Glossary on Mathematical Modeling".	2 2 4
Numerical Methods			
10-14	- Ordinary Differential Equation; - Boundary-value Problems; - Partial Differential Equation.	Test your knowledge: ODEs; Test your knowledge: BVPs; Test your knowledge: PDEs; Assignment "Euler's Method"; Assignment "Runge-Kutta Numerical Schemes"; Assignment "Accuracy and Stability Control of Explicit Methods".	4 1 1 2 2 2 4 4 4
Final exam			
15	- Final test; - Oral exam.		4 4

Lecturer and Contact Information

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Assessment

Grade policy for both home assignments and the final exam is:

- A (excellent work) 91–100 points
- B (above average work) 81–90 points
- C (average work) 71–80 points
- D (below average work) 50–70 points
- F (failed work) < 50 points

To pass the exam students have to do all course's assignments, otherwise they will not be allowed to perform final test. The final exam consists of two parts: a final test and an oral exam.

Students should be able to:

- perform the final test in the online course (30 points maximum),
- give an answer on 2 questions, demonstrate processes' schematic diagrams and explain them (70 points maximum).

Attendance Policy

Students are expected to attend and participate in classes and should notify trainers of excused absences in advance, where possible. Students who have an excused absence are expected to make arrangements with instructors for alternative assignment.

Every topic has a home assignment work that should be done. The final mark will be made by the same grade policy as for a final exam.

Web page of the course

The webpage of the course Mathematical Modeling is available through E-learning SibFU web site: www.e.sfu-kras.ru . You must be logged in to access this course. Course materials and required reading materials are available at the course web-page.

Core reading

The main books for this course are Lecture Notes on Mathematical Modelling in Applied Sciences Nicola Bellomo, Elena De Angelis, and Marcello Delitala (2007) and Mathematical Modeling in Chemical Engineering Von A. Rasmuson, B. Andersson, L. Olsson, R. Andersson (Cambridge University Press, ISBN 978-1-107-04969-7, 2014).

Lecture Notes on Mathematical Modelling in Applied Sciences Nicola Bellomo, Elena De Angelis, and Marcello Delitala (2007). It contains all information that is required for study in a more extensive manner. It will help students to reach a deeper understanding of mathematical modeling.

Mathematical Modeling in Chemical Engineering Von A. Rasmuson, B. Andersson, L. Olsson, R. Andersson (Cambridge University Press, ISBN 978-1-107-04969-7, 2014) provides mathematical models and examples of phenomena in the field of chemical engineering.