Course guide
390338 - MSSB - Modelling and Simulation of Biological Systems

Last modified: 20/07/2023

Unit in charge: Barcelona School of Agri-Food and Biosystems Engineering
Teaching unit: 748 - FIS - Department of Physics.

Degree: BACHELOR'S DEGREE IN BIOSYSTEMS ENGINEERING (Syllabus 2009). (Compulsory subject).

Academic year: 2023 **ECTS Credits:** 6.0 **Languages:** Catalan

LECTURER

Coordinating lecturer: CLARA PRATS SOLER

Others: Alvarez Lacalle, Enrique
Lopez Codina, Daniel

DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES

Specific:
1. Biological models and determination of their main properties.

TEACHING METHODOLOGY

The training activities will include theoretical classes, practical classes and guided activities. The theoretical sessions will consist of lectures and cooperative classes, including practical exercises to be solved with a spreadsheet proposed by the teacher on a topic already worked on, in which a high level of student participation will be promoted. The practices will be done with computers. In these sessions you will work individually or in small groups, and at the end of the sessions you will have to present an individual report on the practice carried out.

LEARNING OBJECTIVES OF THE SUBJECT

Understand the basic foundations of modeling in the field of biological systems engineering, understand existing models and identify the utilities, limitations and areas of application. Use existing simulation programs, adjusting their parameters to experimental data, and interpret the meaning and validity of the results obtained. Design, implement and use new models and simulations following the various stages of the modeling and simulation process.

STUDY LOAD

Type	Hours	Percentage
Hours large group	40,0	26.67
Hours small group	20,0	13.33
Self study	90,0	60.00

Total learning time: 150 h

CONTENTS

FUNDAMENTALS OF MODELLING AND SIMULATION

Description:
1.1 Basic concepts
Science, technology, mathematics and biology. Postulates and principles of science versus models. Need for modeling in science and technology.
1.2 Types of models
Top-down strategy and bottom-up strategy. Continuous models in differential equations. Models in compartments. Models with explicit space. Cellular automaton. Agent-based models. Nets.
1.3 Numerical methods
interpolation Numeric filters. Numerical derivative. Numerical integration. Sensitivity analysis. Parameterization of functions.
1.4 Continuous growth and decline models
Growth models: exponential, logistic, Gompertz and others. Decay models: exponential and others. deterministic chaos
1.5 Introduction to programming
Parameters and variables. Structure of a programming code.

Related activities:
Activity 1: Theoretical explanation classes.
Activity 2: Individual assessment tests.
Activity 3: Practical sessions with computers in the classroom.

Full-or-part-time: 23h
Theory classes: 9h
Laboratory classes: 4h
Self study : 10h

CONTINUOUS MODELS IN BIOCHEMISTRY AND IN MICROBIOLOGY

Description:
2.1 Enzyme kinetics
Michaelis-Menten kinetics
2.2 Primary models
Specific growth rate of a crop. Experimental measurement of the growth curve. Growth phases of a batch culture. Primary models. Model by Baranyi and Roberts.
2.3 Secondary models
Monod's model (substrate concentration). Ratkowsky model (temperature).
2.4 Continuous cultures
Modeling of a simple bioreactor
2.5 Models of inhibition
Non-competitive inhibition. Exponentially decreasing inhibition. Competitive and non-competitive inhibition. Inhibition per substrate. Generalized Monod kinetics
2.6 Tertiary models
ComBase platform

Related activities:
(ENG) Activitat 1: Classes d'explicació teòrica.
Activitat 2: Proves individuals d'avaluació.
Activitat 3: Sessions pràctiques amb ordinadors a l'aula.

Full-or-part-time: 23h
Theory classes: 9h
Laboratory classes: 4h
Self study : 10h

COMPARTIMENTAL MODELS

Description:
3.1 Structure, formalism and representation
3.3 Examples in microbiology and pharmacokinetics
Single-compartment model: use of tracers. Two-compartment model: pharmacokinetics. Models with more compartments: bioreactors with simultaneous processes. Matrix notation.

Related activities:
(ENG) Activitat 1: Classes d'explicació teòrica.
Activitat 2: Proves individuals d'avaluació.
Activitat 3: Sessions pràctiques amb ordinadors a l'aula.

Full-or-part-time: 23h
Theory classes: 5h
Laboratory classes: 2h
Self study : 16h

MODELS WITH EXPLICIT SPACE

Description:
4.1 Models with continuous space
Diffusion modeling. Heat transport by conduction.
4.2 Cellular automaton
The game of life. Applications in environment and physiology.

Related activities:
(ENG) Activitat 1: Classes d'explicació teòrica.
Activitat 2: Proves individuals d'avaluació.
Activitat 3: Sessions pràctiques amb ordinadors a l'aula.

Full-or-part-time: 33h
Theory classes: 5h
Laboratory classes: 4h
Self study : 24h

AGENT-BASED MODELS AND COMPLEX NETWORKS

Description:
5.1 Agent-based and Individual-based models
formalism Agent-based models vs continuous models. Examples in epidemiology and microbiology
5.2 Complex networks in systems biology
Introduction and formalism. Complex networks in systems biology

Related activities:
(ENG) Activitat 1: Classes d'explicació teòrica.
Activitat 2: Proves individuals d'avaluació.
Activitat 3: Sessions pràctiques amb ordinadors a l'aula.

Full-or-part-time: 25h
Theory classes: 3h
Laboratory classes: 4h
Self study : 18h

MATHEMATICAL EPIDEMIOLOGY

Description:
6.1 Introduction
Descriptive epidemiology. Conceptual relations with ecology. R strategy and K strategy. Mathematical models in epidemiology. Incidence, prevalence, control, elimination, eradication and extinction.
6.2 Models structured in compartments
SI model, SIS model, SIR model, SIRS model, SEIR model, other models. Basic and effective reproductive speed. Severity of a disease.
6.3 Diseases of vector transmission
SIR models with vector transmission.
6.4 IbM models and complex networks in epidemiology
Individual-based models. Complex networks in epidemiology.

Related activities:
(ENG) Activitat 1: Classes d'explicació teòrica.
Activitat 2: Proves individuals d'avaluació.
Activitat 3: Sessions pràctiques amb ordinadors a l'aula.

Full-or-part-time: 20h
Theory classes: 6h
Laboratory classes: 2h
Self study : 12h

DEVELOPMENT OF MODELS

Description:
Implications of physics in the development of models of biological systems
Concepts and vocabulary of thermodynamics. Conservation principles. Second principle of thermodynamics.
7.2 Model development methodology
Methodology. Scope of application of the various types of models.

Full-or-part-time: 5h
Theory classes: 3h
Self study : 2h

ACTIVITIES

(ENG) CLASSES D'EXPLICACIÓ TEÒRICA

Full-or-part-time: 88h
Theory classes: 38h
Self study: 50h

(ENG) PROVES INDIVIDUALS D'AVALUACIÓ

Full-or-part-time: 2h
Theory classes: 2h

PRACTICAL SESSIONS

Description:
Practice 0: Introduction to programming with Matlab
Practice 1: Introduction to programming with Matlab (II)
Practice 2: Historical growth models
Practice 3: Simulation of a bioreactor
Practice 4: Pharmacokinetics models
Practice 5: Spread of the Chagas disease vector in a community
Practice 6: Modeling based on the individual of a bacterial culture
Practice 7: Propagation of the action potential in cardiac tissue
Practice 8: The cell makes a decision
Practice 9: Flu epidemic in an English boarding school

Material:
Laptops of students

Delivery:
Report of practices P1 to P9 through Atenea

Full-or-part-time: 60h
Laboratory classes: 20h
Self study: 40h

GRADING SYSTEM

N1: The practical reports delivered to the teacher will be corrected and evaluated.
N2: There will be two exams (partial and final) that will consist of two tests each (theoretical-practical and practical), and that will make up 75% of the final grade.
Nfinal = 0.25N1 + 0.75N2

EXAMINATION RULES.

PRACTICAL SESSIONS AND REPORTS:
1) The practical sessions are designed as face-to-face, as they require the supervision and support of the teacher. Therefore, practice items will only be evaluated if the student attends the corresponding sessions. In duly justified cases, the practice may be done without having attended the corresponding session and prior notification to the teacher. In these cases, the grade of the initial questions of that session will not be taken into account in the calculation of the final grade.
2) Reports must be done individually, although you can count on the occasional support of colleagues, in order to guarantee the correct progress in the learning process of all students. If a copy is detected between students of the same course or with respect to previous courses, a 0 will be added to the overall practical sessions qualification (N1).
3) Reports must be submitted within the deadlines indicated in Atenea. No deliverables will be accepted beyond December 30.

EXAMS:
1) Exams must be taken individually and without any support from the teacher or other students. Therefore, if a copy is detected, the students involved will be assigned a 0 for the subject. Notes and forms cannot be taken to the theory block. For the practical block, you can take a sheet written on both sides with the diagrams or lists of orders that the students consider necessary.

BIBLIOGRAPHY

Basic:
- Haefner, James W. Modeling biological systems : principles and applications [on line]. 2nd ed. New York: Springer, cop. 2005 [Consultation: 31/10/2023]. Available on: https://ebookcentral-proquest-com.recursos.biblioteca.upc.edu/lib/upcatalunya-ebooks/detail.action?pq-origsite=primo&docID=6311640. ISBN 0387250115.