Universitat Autònoma de Barcelona

2017/2018

Modelling and Simulation of Biosystems.

Code: 100919
ECTS Credits: 6

Degree	Type	Year	Semester
2500253 Biotechnology	OT	4	0

Contact

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Use of languages

Principal working language: catalan (cat)

Some groups entirely in English: No

Some groups entirely in Catalan: Yes

Some groups entirely in Spanish: No

Prerequisites

To have fundamental knowledge of algebra, differential and integral calculus, chemistry and biochemistry.

Be able to read English scientific literature.

Be able to use basic office software (word, Excel,...)

Basic knowledge in computer programming is an advantage

Oral and written basic knowledge of Catalan language is necessary

Objectives and Contextualisation

Computer simulation of real systems is a well-developed field of science especially in engineering areas, in physics or in chemistry. In biotechnology and in generally in biological sciences, its application was initially limited. In this context classical simulation approaches reproduce the behavior of microorganisms and enzymes in bioreactor. But the real impact of computer simulation in biotechnology results as a consequence on one side, due to the accumulation of knowledge about the isolated operation of components of biological systems and on the other side from the experimental observation that the components of a biological entity, such as a cell, operate in an autonomous and coordinated manner as an integrated system. Thus the biological system can be seen as a network of networks (metabolic, genetic, signal transduction,..) operating in a coordinated manner. This way, to understand the operation of even one of the simplest of those systems, is not possible without the perspective of its operation as an integrated system. The operation as a system results in the emergence of key properties, non-existing in any of its isolated parts but fundamental for the successful operation of the system. This new vision has resulted in the emergence of the field of Systems Biology. Biological systems computer simulation has been key in the development of systems biology, together with the increasing accumulation of knowledge on the operation of biological systems in public databases and the wide spread and cheap availability of computing power. By means of computer simulation it is made evident the different behaviors obtained depending on the individual properties of the components, their interconnections as well as the operational conditions.

In this context the course intends to introduce the student in the basic approximations and methodologies to simulate the behavior of a biological system in a computer. From the bioreactor as an experimental system to the examples of simulation of different types of networks (metabolic, genetic, signal transduction,..) in different operational modes (steady state, dynamic,..). As a global objective it is intended that the student has a firsthand experience on the differences and relevance of the behavior of a system as an integrated 'whole' in opposition to the isolated characteristics of its components, as well as the information derived from the different operational modes and therefore the requirements for their study.

As the main goal is to offer the student firsthand experience on biological systems simulation, the course has a high practical content. Thus the student will use either a programming environment, such as Matlab, to understand the basic procedures by means of simple examples, as well as using more specific simulation software for biological systems (SBW, COPASI, ...) in examples of higher complexity.

The different subjects are introduced gradually, from the basic concepts towards the description of systems of increasing complexity. In a way such that the student can understand the need to study biological systems as integrated entities in the context of the new biotechnology of the XXI century.

Content

1. Introduction. Models and systems
    1. Model. Definition, advantages, necessity
    2. Approximations to systems modelling
    3. Characteristics of systems
    4. Phases in the modelling process
    5. Components and types of models.
2. Review of fundamental concepts and modelling
    1. Balance equations and structure.
    2. Kinetics and thermodynamics
3. Dynamics of simple systems
    1. Bioreactor and biocatalyst systems
    2. Simple metabolic systems
    3. Basics of systems dynamics
4. Systems in steady state
    1. Bioreactor and biocatalyst systems
    2. Metabolic networks. Elementary modes.
    3. Optimization of systems in steady state.
    4. Systems sensitivity analysis. Metabolic control theory
6. Simulation examples
    1. Metabolic networks
    2. Gene networks.
    3. Signal transduction networks