

## Advanced Biosystems Modelling (I003021)

**Course size** *(nominal values; actual values may depend on programme)*

**Credits 5.0**

**Study time 150 h**

**Course offerings in academic year 2024-2025**

A (semester 2)

English

Gent

**Lecturers in academic year 2024-2025**

Van Liedekerke, Paul

LA26

lecturer-in-charge

Baetens, Jan

LA26

co-lecturer

**Offered in the following programmes in 2024-2025**

Master of Science in Bioscience Engineering: Cell and Gene Biotechnology	5	A
Master of Science in Bioscience Engineering: Chemistry and Bioprocess Technology	5	A
Master of Science in Bioscience Engineering: Environmental Technology	5	A
Master of Science in Bioscience Engineering: Food Science and Nutrition	5	A
Master of Science in Pharmaceutical Engineering	5	A
Exchange Programme in Bioscience Engineering: Cell and Gene Biotechnology (master's level)	5	A
Exchange Programme in Bioscience Engineering: Chemistry and Bioprocess Technology (master's level)	5	A
Exchange Programme in Bioscience Engineering: Environmental Technology (master's level)	5	A
Exchange Programme in Bioscience Engineering: Land and Forest management (master's level)	5	A

**crdts**

**offering**

**Teaching languages**

English

**Keywords**

Partial Differential Equations (PDEs), Numerical schemes and stability, Computational Fluid Dynamics (CFD), Spatial-temporal Models, Agent-based Models (ABM), Ecological Models, Cell-Based Models.

**Position of the course**

Many processes in nature and bio-engineered systems are complex and are constituted of elements that are both discrete and continuous in nature. Think about, for example, the spread of species in an ecological system, the propagation of infectious diseases, or the hydrodynamics in bioreactors. To understand these processes, one must use appropriate modelling techniques. The goal of this course is to give the future bio-engineer insights into currently used and advanced simulation methods that are designed to understand and predict spatial-temporal phenomena present in many biosystems. The course starts an analysis of PDEs and introduces the students to established numerical schemes that are generally applicable. The second part of the course introduces Computational Fluid Dynamics (CFD), whereby the focus will be on engineered biosystems, and the students will learn to work with a commercial software package. The third part of the course addresses the modelling of systems that are discrete in nature, for example, Agent-based models that are used to simulate and predict the complex emergent behaviour of many species (cells, organisms) and their interactions.

**Contents**

**Part A - Partial differential equations and numerical solution methods**

1 Introduction to partial differential equations: types of PDEs: diffusion problems,

hydodynamics (Navier-Stokes), waves

2 Solution methods to PDEs and numerical schemes: Finite Differences and Finite Volumes (exercises in Python)

3 Implement the Navier-Stokes Equations using the Finite Differences approach.

### **Part B – Computational fluid dynamics**

1 General introduction to CFD (meshing, solver setup, simulation, and post-processing)

2 Use CFD using Ansys Fluent, using the Finite Volume Method.

3 Introduction to turbulence modelling (RANS)

4 Case study: study of flow and hydrodynamics in bioreactor or study of fluid flow in pipes.

### **Part C – Spatially explicit modelling paradigms for discrete systems**

1 Discrete Element Methods (DEM): introduction and applications (granular matter dynamics)

2 Agent-Based Models (ABM): techniques and applications (tumor growth, organoids,...)

3 Cellular automata: techniques and applications (dynamics of eco-systems, disease spreading, ...)

### **Initial competences**

The course heavily draws on the knowledge acquired in the courses : Differential Equations and Modelling and Simulation of Biosystems (ModSim)

Prior knowledge list:

- Ordinary differential equations (analysis and numerical solutions), Fourier series and transforms.
- Experience with Python or other programming language is recommended
- Good knowledge of algebra and calculus

### **Final competences**

- 1 Being able to translate complex systems into mathematical models for bioprocesses including (bio)kinetics, transport phenomena or particle-particle interactions.
- 2 Able to Implement and apply numerical solvers to solve PDEs (in Python) and critically interpret the results.
- 3 Having basic knowledge of CFD simulations and experience with commercial CFD software (Ansys)
- 4 Understanding how Discrete Modelling works (DEM, ABMs), where they can be used, and what are the advantages and limitations.

### **Conditions for credit contract**

Access to this course unit via a credit contract is determined after successful competences assessment

### **Conditions for exam contract**

This course unit cannot be taken via an exam contract

### **Teaching methods**

Seminar, Lecture

### **Extra information on the teaching methods**

- Theory: course notes (syllabus)
- Python notebooks are used to learn and implement the methods.
- A commercial CFD package with graphical user interface will be used to build the models and simulate flows.

### **Study material**

Type: Laptop

Name: Python notebooks / CFD software

Indicative price: Free or paid by faculty

Optional: no

### **References**

H. Versteeg, W. Malalasekera (2007): An Introduction to Computational Fluid Dynamics: The Finite Volume Method.

### **Course content-related study coaching**

**Assessment moments**

end-of-term and continuous assessment

**Examination methods in case of periodic assessment during the first examination period****Examination methods in case of periodic assessment during the second examination period**

Oral assessment, Assignment

**Examination methods in case of permanent assessment**

Oral assessment, Assignment

**Possibilities of retake in case of permanent assessment**

examination during the second examination period is possible in modified form

**Extra information on the examination methods**

Discuss a scientific paper (numerical method, or a method in general)

Project: Build a CFD model in Ansys

**Calculation of the examination mark**