



[30h+15h exercises] 4 credits

This course is taught in the 2nd semester

**Teacher(s):** Denis Dochain, Fernand Thyrion

**Language:** french

**Level:** 2nd cycle course

## Aims

Introduction to simulation techniques, to flowsheeting and to process optimisation.

## Main themes

### 1) Basic concepts

General structure and operating mode of a process simulation software. Flowsheeting methods. Evaluation and selection of thermodynamic, kinetic and unit operation models.

### 2) Mathematical tools

Numerical methods of integration of partial differential equations used in chemical engineering. Finite difference methods, Weighted residuals methods (orthogonal collocation).

### 3) Numerical simulation

Solution of a simulation flowsheet. Operation principles of a software (ASPEN). Generation of thermodynamic properties, use of a software for the design of equipments and the parameter sensitivity study. Simulation of the most important unit operations.

### 4) Optimisation

Application of optimisation methods to typical processes like heat exchangers, reactor cascade, distillation columns,#

Applied methods : nonlinear optimisation with constraints (e.g. generalised reduced gradient, sequential quadratic programming, Lagrange multipliers,#)

## Other credits in programs

<b>BIR22/2C</b>	Deuxième année du programme conduisant au grade de bio-ingénieur : Chimie et bio-industries (Ingénierie biomoléculaire et cellulaire)	(4 credits)	Mandatory
<b>INCH22</b>	Deuxième année du programme conduisant au grade d'ingénieur civil chimiste	(4 credits)	Mandatory