UAB
Universitat Autònoma de Barcelona

Simulation of Chemical Processes

Code: 102444
ECTS Credits: 3

2024/2025

Degree	Type	Year
2500897 Chemical Engineering	OB	3

Contact

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Teaching groups languages

You can view this information at the end of this document.

Prerequisites

It is recommended to have taken the following subjects:

- Applied thermodynamics
- Chemical Reactors
- Heat transfer
- Fluid transport and circulation
- Separation operations
- Chemical kinetics
- Computer applications

Objectives and Contextualisation

1. Learn how to optimally use commercial process simulation tools.
2. Acquire the simulation knowledge necessary to pose and solve paradigmatic cases of Chemical Engineering, especially those that need advanced mathematical tools for solving their matter and energy balances, both in steady state and in non-steady state.
3. Apply simulation tools to predict the behavior of processes.
4. Acquire the necessary knowledge to carry out parameter sensitivity analyzes through mathematical simulation.
5. Application of process parameter optimization algorithms

Competences

- Apply the techniques for analysing and synthesising systems to process and product the engineering.

- Demonstrate basic knowledge of the use and programming of computers, and apply the applicable IT resources to chemical engineering.
- Demonstrate knowledge of the different reaction, separation and processing operations for materials, and transport and circulation of fluids involved in the industrial processes of chemical engineering.
- Demonstrate understanding of the main concepts for controlling chemical engineering processes.
- Develop personal work habits.
- Work in a team.

Learning Outcomes

1. Apply IT resources to the simulation and control of processes.
2. Apply knowledge of separation operations and reactors to the preparation of models and to the simulation of processes.
3. Create models of the dynamic behaviour of compound systems for a variety of operations.
4. Use mathematical models of dynamic systems and processes in the field of chemical engineering.
5. Work autonomously.
6. Work cooperatively.

Content

1. Introduction to the subject
   2. Review of Optimization concepts. Process Simulation Applications
   3. Commercial simulation tools for equipment and process design
   4. Simulation of steady state processes:
   4.1 Estimation of properties of pure compounds and mixtures

   4.2 Applied thermodynamics

   4.3 Heat transmission and exchangers

   4.4. Chemical kinetics and ideal reactors

Activities and Methodology

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Hands-on session Block 2	4	0.16	1, 2, 3, 4, 5
Hands-on session Block 4	16	0.64	1, 2, 3, 4, 5
Seminars	4	0.16	1, 2, 3, 4
Theoretical lessons	7	0.28	2, 3, 4
Type: Autonomous			
Individual work	40	1.6	1, 2, 3, 4, 5, 6

The subject is structured in three types of sessions:

- 12 theoretical-practical sessions (100 minutes) held in the IT classrooms where the theoretical content will first be presented and then applied in the practical part of the session, where the students will work in pairs. Some of the built cases may be non-evaluable deliverables
- 2 Evaluable practical sessions (2 h) held in the computer classrooms, in which the students, individually, will solve problems from thematic blocks 2; 4.1 + 4.2 + 4.3 + 4.4. At the end of the session, the students submit the results obtained and are evaluated.
- 2 Seminars (90 minutes) given by experts in the field of commercial process simulation (external to the UAB)

The evaluable activity corresponding to block 2 will count for 30% of the total grade

The evaluable activity corresponding to blocks 4.1 + 4.2 + 4.3 + 4.4 will count for 60% of the total grade

Attendance at each of the seminars taught by external experts will count for 5% of the total grade

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Assessment

Continous Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Assessed activity Block 2	30%	2	0.08	1, 2, 5
Assessed activity Blocks 4.1 + 4.2 + 4.3 + 4.4	60%	2	0.08	1, 2, 5
Attendance to seminars	10%	0	0	1, 2, 3, 4, 5, 6
Make-up final exam	100%	0	0	1, 2, 3, 4, 5

a) Continuous evaluation:

The subject is assessed continuously with 2 individually assessable activities, one with the contents of block 2 (which accounts for 30% of the total), and another with the contents of blocks 4.1 + 4.2 + 4.3 + 4.4 (which accounts for a 60% of the total). These activities will take the form of a partial exam in the computer labs. On the other hand, attendance at each of the 2 seminars taught by experts external to the UAB will count for 5% of the total.
In the case of irregularities in any of these assessable activities, the criteria of point e) will be applied.
To pass the subject, you will need to get a minimum of 5.0 as an average grade in the continuous assessment and a minimum grade of 3.0 in each assessable activity.
b) Review of qualifications:

For each assessment activity, a review place, date and time will be indicated in which the student can review the activity with the teacher. In this context, claims can be made about the grade of the activity, which will be evaluated by the teaching staff responsible for the subject. If the student does not appear for this review, this activity will not be reviewed later.

c) Recovery:

The student who does not pass the subject through the continuous assessment may take a final remedial exam, which will include content from the entire subject and which will count for 90% (10% of the attendance at the seminars will be kept).

The minimum grade to pass this final exam is again 5.0. In the case of not appearing for this exam, the student will keep the grade of the continuous assessment (whatever it is).

The student can present himself for recovery as long as he has presented himself to a set of activities that represent a minimum of two-thirds of the total grade of the subject.

d) Qualifications:

Honor matriculations. Awarding an honors matriculation qualification is the decision of the teaching staff responsible for the subject. UAB regulations indicate that MH can only be granted to students who have obtained a final grade equal to or higher than 9.00. Up to 5% of MH of the total number of enrolled students can be awarded.

A student will be considered non-evaluable (NA) if he has not taken part in a set of activities whose weight is equivalent to a minimum of two-thirds of the subject's total grade.

e) Irregularities by the student, copying and plagiarism:

Without prejudice to other disciplinary measures deemed appropriate, irregularities committed by the student that could lead to a change in the grade of an assessment act will be graded with a zero. Therefore, copying, plagiarism, deception, copying, impersonation, etc. in any of the assessment activities will involve failing it with a zero. Assessment activities qualified in this way and by this procedure will not be recoverable. If it is necessary to pass any of these assessment activities to pass the subject, this subject will be suspended directly, with no opportunity to recover it in the same course. In this case, the student's final grade is a FAIL (3.0 numerical grade).

f) Calendar and schedule:

The dates of continuous assessment and assignment of assignments will be published in the corresponding Moodle classroom and may be subject to possible changes in programming for reasons of adaptation to possible incidents. You will always be informed via the Moodle classroom about these changes as it is understood that this is the usual platform for exchanging information between teachers and students.

This subject does not provide for a single assessment system.

Bibliography

Manuals and help for the software used

- Aspen Physical Property Methods V12 (October 2020)
- Aspen Physical Property Models V12 (October 2020)
- Aspen HYSYS. Unit Operations Reference Guide V12.1 (May 2021)

Specific bibliography of the cases considered

- Foo, D., "Chemical Engineering Process Simulation", 2nd Edition (2022)
- Edgar, T. F., et al. « Optimization of Chemical Processes », 2nd Edition (2001)
- Turton, R., "Analysis, Synthesis, and Design of Chemical Processes, 5th Edition (2019)
- Hanyak Jr., M.E., "Chemical Process Simulation and the Aspen HYSYS software" (2012)

Software

The various programmes contained in the AspenTech suite (aspenONE) will be used

Optionally, you can use Matlab and MS Excel in some optimization exercise

Optionally, a seminar with other commercial simulators will be offered.

Language list

Name	Group	Language	Semester	Turn
(PAUL) Classroom practices	211	Catalan	second semester	morning-mixed
(PAUL) Classroom practices	212	Catalan	second semester	morning-mixed
(PAUL) Classroom practices	213	Catalan	second semester	morning-mixed
(PAUL) Classroom practices	214	Catalan	second semester	morning-mixed