Universitat Autònoma de Barcelona

2023/2024

Simulation of Chemical Processes

Code: 102444
ECTS Credits: 3

Degree	Type	Year	Semester
2500897 Chemical Engineering	OB	3	2

Contact

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Teaching groups languages

You can check it through this link. To consult the language you will need to enter the CODE of the subject.
Please note that this information is provisional until 30 November 2023.

External teachers

Josep Anton Feliu Gil

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. Reinforce the bases that govern the main processes of Chemical Engineering: material and energy balances in steady and non-steady state.
2. Learn commercial process simulation tools.
3. Acquire the simulation skills necessary to pose and solve paradigmatic cases in Chemical Engineering, especially those that require advanced mathematical tools for their resolution.

4. Apply simulation techniques to predict the behaviour of processes.

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. Simulation tools for equipment and process design.
2. Simulation of steady state processes:

   2.1 Applied thermodynamics. Estimation of the properties of pure components and mixtures
   2.2 Chemical kinetics and ideal reactors
   2.5 Separation processes

Methodology

The course is structured in four types of sessions:

- 8 theoretical sessions (1 h) carried out in class where the cases that will be studied in the practical sessions will be presented.
- 4 non-assessable practical sessions (2 h) held in the computer classrooms, in which students, in pairs, carry out a practical example of one of the blocks.
- 2 assessable practical sessions (2 h) held in the computer rooms, in which students, individually, carry out a practical example of each of the blocks. At the end of the session, the students hand in the results obtained and are evaluated.
- 2 seminars (1 h) led by experts in the field of commercial process simulation (external to the UAB).

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.

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Theoretical classes	8	0.32	2, 3, 4
Type: Supervised			
Non-assessable session Block 2.1	2	0.08	2, 1, 3, 5, 4
Non-assessable session Block 2.2	2	0.08	2, 1, 3, 5, 4
Non-assessable session Block 2.5	2	0.08	2, 1, 3, 5, 4
Seminars	2	0.08	2, 1, 3, 4
Type: Autonomous			
Individual work	50	2	2, 1, 3, 6, 5, 4

Assessment

a) Continuous assessment:
The subject is assessed on a continuous basis with 2 evaluable activities Blocks 2.1 + 2.2 (45%) and Block 2.5 (45%) plus 10% for attendance at the 2 seminars.
The activities of Blocks 2.1 + 2.2 and 2.5 will take the form of a partial exam in the computer classrooms.
In the case of irregularities in any of these evaluable activities, the criteria of point e) will be applied.
In order to pass the subject it will be necessary to obtain a minimum mark of 5.0 as an average mark in the continuous assessment and a minimum mark of 1.0 in each activity, except in the case that the student does not attend the activity.

b) Review of qualifications:
For each assessment activity, a place, date and time of review will be indicated in which the student can review the activity with the teacher. In this context, claims can be made on the mark for the activity, which will be assessed by the lecturer responsible for the subject. If the student does not attend this review, this activity will not be reviewed later.

c) Recovery:
Students who do not pass the course by means of continuous assessment (whether they have a Fail or a Non-assessable) may take a final make-up exam, which will include any part of the course and which will count for 100%. Students who have passed in order to improve their marks can also take the make-up exam, but they will then renounce the grade of the continuous assessment.
Any student who sits this exam automatically gives up any previous qualification s/he may have had on a continuous basis. The minimum mark for passing this final exam is again 5.0. If the student does not take this exam, he/she will keep the grade of the continuous assessment (whatever it is).
Students may sit the make-up exam provided they have taken a set of activities that represent a minimum of two thirds of the total grade for the course.

d) Qualifications:
Matricula d'honor. The decision to award an honours qualification is the decision of the lecturers responsible for the course. UAB regulations state that MHs can only be awarded to students who have obtained a final grade of 9.00 or higher. Up to 5% of the total number of students enrolled may be awarded MHs.
A student will be considered not assessable (NA) if he/she has not taken part in a set of activities, the weight of which is equivalent to at least two thirds of the total qualification of the course.

e) Irregularities on the part of the student, copying and plagiarism:
Without prejudice to other disciplinary measures that may be deemed appropriate, irregularities committed by the student that may lead to a change in the grade of an assessment act will be graded with a zero. Therefore, copying, plagiarism, cheating, allowing copying, etc. in any of the assessment activities will result in a fail mark of zero. Assessment activities graded in this way and by this procedure will not be recoverable. If it is necessary to pass any of these assessment activities in order to pass the course, this subject will be failed directly, with no opportunity to make it up in the same course. In this case, the student's final mark will be a fail (3.0 numerical grade).

f) Calendar and programming:
The dates of continuous assessment and work delivery will be published in the corresponding Moodle classroom and may be subject to possible changes in the programme for reasons of adaptation to possible incidents. Students will always be informed of these changes via the Moodle classroom as it is understood that this is the usual platform for exchange of information between teachers and students.

g) Assessment of repeating students:
Repeating students who have taken the previous subject based on Matlab will be eligible for an evaluation of the contents of previous courses with a final exam that will count 100% of the grade.

This subject does not have a single assessment system.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Assessed activity Block 2.1 + 2.2	45%	2	0.08	2, 1, 3, 5, 4
Assessed activity Block 2.5	45%	2	0.08	2, 1, 3, 5, 4
Attendance to seminars	10%	2	0.08	2, 1, 3, 6, 5, 4
Make-up exam	100%	3	0.12	2, 1, 3, 5, 4

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)
- 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, a seminar with other commercial simulators will be offered.