Universitat Autònoma de Barcelona

2022/2023

Simulation of Chemical Processes

Code: 102444
ECTS Credits: 3

Degree	Type	Year	Semester
2500897 Chemical Engineering	OB	3	2

Contact

Name: Antoni Sanchez Ferrer
Email: antoni.sanchez@uab.cat

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

It is recommended that you have completed the following subjects:

- Chemical reactors
- Transmission of heat
- Separation operations
- Chemical kinetics
- Computer applications

Objectives and Contextualisation

Reinforce the bases that govern the main processes of Chemical Engineering: balance of matter and energy in st
Learn process simulation tools, especially Matlab and Hysys.
Acquire the necessary simulation skills to solve and solve paradigmatic c
Apply the simulation tools to predict the behavior of processes.
Acquire the knowledge necessary to carry out analyzes of sensitivity of p
Optimization.

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

2. Thematic blocks:
   2.1. Chemical kinetics
   2.2. Systems in non-stationary state.
   2.3. Reactors: non-isothermic systems and modeling and simulation of
   2.4. Optimization
3. Simulation of complex systems with Hysys (to be confirmed).

Methodology

The subject is structured with three types of sessions:

- Theoretical sessions (1 hour) done in class where the cases will be presented that will be studied in the practical sessions.

- Non-evaluable practical sessions (2 hours) made in computer rooms, in which the students, individually in the case of the thematic blocks 2.1, 2.2 and 2.3, make a practical example of some of the blocks. Block 3 will be in the form of a group session by an external professor, although it is still to be confirmed.

- Assessable practical sessions (2 hours) done in the computer rooms, in which the students, individually in the case of the thematic blocks 2.1, 2.2 and 2.3, make a practical example of each one of the blocks. At the end of the session, students deliver the results obtained and are evaluated.

- The evaluable session of Block 2.4 consists of an individual optimization work that students will prepare and present in class randomly. The work will be evaluated later.

The evaluable activities of blocks 2.1, 2.2, 2.3 and 2.4 will count for a percentage of 25% of the final mark and are not recoverable.

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			
Session 2.1	2	0.08	2, 1, 3, 5, 4

Session 2.1 (non evaluation)	2	0.08	2, 1, 3, 5, 4
Session 2.2	2	0.08	2, 1, 3, 5, 4
Session 2.2 (non evaluation)	2	0.08	1, 3, 5
Session 2.3	2	0.08	2, 3, 6, 4
Session 2.3 (non evaluation)	2	0.08	2, 1, 3, 5, 4
Session 2.4	2	0.08	2, 1, 3, 6, 4
Session 3 (non evaluation)	2	0.08	1, 3, 5
Type: Autonomous			
Individual work	40	1.6	2, 1, 3, 6, 5, 4

Assessment

Evaluation

a) Continuous evaluation:

The subject is evaluated continuously with 4 evaluable activities of Blocs 2.1, 2.2, 2.3 and 2.4 respectively, which compose 25% each.

The activities of Blocs 2.1, 2.2 and 2.3 will be done in the form of a partial exam in computer laboratories, while the activity evaluated in Block 2.4 will be in the form of work.

In the case of irregularities in any of these evaluated activities, the criteria of point e) will be applied.

To pass the subject, a minimum of 5.0 will be required as the average mark of the continuous evaluation and a minimum score of 1.0 in each activity, except in case the student is not present in the activity.

b) Review of qualifications:

For each assessment activity, a place, date and time of revision will be indicated in which the student will be able to review the activity with the teacher. In this context, claims can be made about the activity note, which will be evaluated by the teachers responsible for the subject. If the student does not submit to this review, this activity will not be reviewed later.

c) Recovery:

The student who does not pass the subject through the continuous evaluation (already has Suspended or has a Non-Evaluable) will be able to do a final examination of recovery, that will include any part of the subject and that will compute by a 100%. The students of the approved test will also be able to take the recovery test to make a note, but then renounce the grade of the continuous evaluation.

Any student who is present at this exam automatically renounces any previous qualifications that he has continuously. The minimum mark to pass this final exam is 5.0 again. In the case of not presenting to this exam the student will keep the note of the continuous evaluation (whatever it is).

The student can submit to the recovery whenever it has been presented to a set of activities that represent a minimum of two thirds of the total grade of the subject.

d) Qualifications:

Honor enrollments Granting an honorific matriculation qualification is a decision of the faculty responsible for the subject. The regulations of the UAB indicate that MH can only be awarded to students who have obtained a final grade of 9.00 or more. It can be granted up to 5% of MH of the total number of students enrolled.

A student will be considered non-evaluable (NA) if it has not been presented in a set of activities whose weight equals to a minimum of two thirds of the total grade of the subject.

e) Irregularities by the student, copy and plagiarism:

Without prejudice to other disciplinary measures considered appropriate, the irregularities committed by the student that can lead to a variation in the rating of an evaluation act will be qualified with a zero. Therefore, copying, plagiarizing, cheating, copying, etc. In any of the assessment activities it will imply suspending 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, without opportunity to recover it in the same course. In this case, the final mark of the student is a SUSPENS (3.0 number rating).
f) Calendar and programming:

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

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Activity 1	25%	2	0.08	2, 1, 3, 5, 4
Activity 2	25%	2	0.08	2, 1, 3, 5, 4
Activity 3	25%	2	0.08	2, 1, 3, 6, 4
Activity 4	25%	2	0.08	2, 1, 3, 5, 4
Recuperation exam	100%	3	0.12	2, 1, 3, 5, 4

Bibliography

Guides

Brian H. Hahn, Daniel T. Valentine. Essential Matlab for Engineers and Scientists (Fourth Edition). Elsevier Ltd.

Simulation:

Finlayson, B.A., (2006), Introduction to chemical engineering computing. Wiley.

Elnashaie S., Uhlig F., (2007), Numerical Techniques for Chemical and Biological Engineers Using MATLAB. Springer.

Cutlip, M.B., Shacham, M., (2008), Resolución de problemas en Ingenieria Química y Bioquímica con Polymath, Excel y Matlab. Prentice Hall.

Cases:

Scott Fogler, H., "Elements of Chemical Reaction Engineering". 4th ed. (2005).

Scott Fogler, H., "Elementos de Ingeniería de las Reacciones Químicas". 4a ed. (2008).

Levenspiel, O., "Chemical reaction engineering". 3rd ed. (1999).

Levenspiel, O., "Ingeniería de las reacciones químicas". 3a ed. (2006).

Missen, R., "Introduction to chemical reaction engineering and kinetics". (1998).

Software

Matlab.