Universidad Zaragoza

Academic Year/course: 2024/25

66212 - Simulation and Optimization of Chemical Processes

Syllabus Information

Academic year: 2024/25
Subject: 66212 - Simulation and Optimization of Chemical Processes
Faculty / School: 110 - Escuela de Ingeniería y Arquitectura
Degree: 531 - Master's in Chemical Engineering
ECTS: 6.0
Year: 1
Semester: First semester
Subject type: Compulsory
Module:

1. General information

Simulation and optimisation of chemical processes (process analysis) is based in the use of advanced calculations and mathematical models as well as IT tools in order to predict the behaviour of a system. Considering the power of the simulation as a predictive tool, it can be used in design, alternative differentiation, cost calculation, operation, energetic optimisation, safety and risk analysis, logistics and a long etcetera.

2. Learning results

- To perform the mathematical modelling of phenomena and process units that are usual in chemical engineering, as well as of the interactions between the different units of a system (process flow diagram). To be able to choose the most adequate simulation scale for the interests of the previously set target.
- To be able to choose acceptable simplifications based on the destination of the modelling results. To be able to choose an adequate balance between “detail-precision” and “robustness-resolution economy”.
- To be able to solve simulation models of units and processes using ad hoc calculation tools. To be able to use commercial calculation programs with the same purpose. In addition, to be able to adequate the tool used to the complexity level, availability and circumstances.
- To know the process optimisation technique that is more adequate to the typology, complexity of the problem to be solved and to apply it.
- To correctly analyse the results obtained in the simulation-optimisation. To be critical with the results and assign them a validity/uncertainty level.

3. Syllabus

BLOCK A.- SIMULATION

1. Models and Systems. Process Analysis.

2. Block, flowsheet and P&ID diagrams.

3. Tear streams, loops and solving strategies.

4. Models for the estimation of thermodynamic and fluiddynamic properties.

5. Auxiliary unit models.

6. Conceptual reactors' models.

7. Ideal reactors' models.

8. Separation units I: Phase splitters.

9. Separation units II: Rectification and absorption/stripping.

10. Heat exchangers' models.

11. Dynamic simulation of process units.

12. Introduction to cost estimation.

BLOCK B.- OPTIMIZATION OF CHEMICAL PROCESSES

13. Introduction to process optimisation.

14. non-lineal optimisation.

15. Lineal optimisation.

16. Advanced optimisation techniques.

17. Optimisation of heat exchanger networks.

18. Dynamic optimisation of process units.

4. Academic activities

Foreword:

This subject is English Language Friendly (ELF) in at least one group. The study and class material is available in English and the teachers will attend office hours and prepare and evaluate students in English if they don't speak Spanish.

Typology of classes:

Master classes (**30 h**) where the theory of the different topics will be taught.

Face-to-face problem solving and case studies classes (**20 h**).

Practical laboratory sessions (**8 h**) where, through practical exercises, the student will reinforce the contents covered in the master classes.

Special practice session (**2 h**) corresponding to a visit to a company, expert talk, thematic seminar or similar.

Tutored works (**6** non-face-to-face hours) individually or in groups. 1 or 2 activities will be proposed, tutored by the teachers.

Practical research and application works. (**18** non-face-to face hours). where a group of 2-3 students must solve a large scale problem.

Individual study (**60** non-face-to-face hours).

Assessment (**6 h**). There will be a global test.

5. Assessment system

Option 1: *Continuous assessment*

This option includes:

1. Solving the proposed problems and cases (**CPP**) Class attendance and participation.
2. Tutored works (**TTE**) 1-2 individual tasks per academic year.
3. Large-scale practical exercise (Final project) (**TFC**) It will be done in groups of 2-3 students.
4. Completion of a final exam (**EXA**) at the end of the subject. This test will be an “open book” one and will consist of practical exercises that must be solved using the resources that the student deems appropriate (books, notes, data tables, calculator, etc.)- The test must be solved individually.

The grade of the subject will be calculated according to the following weighting:

Grade = 0.1× ***CPP*** + 0.1 × ***TTE*** + 0.2 ***TFC*** + 0.6 × ***EXA***

All the assessment categories will be graded out of 10 points. A minimum grade of 4 out of 10 in the exam (**EXA**) will be required to pass the subject.

Points 1-3 will only be assessable during the teaching period of the subject.

Option 2: *Global assessment*

The final grade will only be that of the exam (**EXA**) The grade will be out of 10 and will offer the student to do some extra exercise to assess the acquisition of the skills corresponding to **TTE** and **TFC.**

Grade = 1.0 × **EXA**

Options 1 and 2 are mutually exclusive.

6. Sustainable Development Goals

7 - Affordable and Clean Energy
9 - Industry, Innovation and Infrastructure
12 - Responsible Production and Consumption