Universidad Zaragoza

66212 - Simulation and Optimization of Chemical Processes

Información del Plan Docente

Academic Year	2018/19
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

1.1.Aims of the course

1.2.Context and importance of this course in the degree

1.3.Recommendations to take this course

2.Learning goals

2.1.Competences

2.2.Learning goals

2.3.Importance of learning goals

3.Assessment (1st and 2nd call)

3.1.Assessment tasks (description of tasks, marking system and assessment criteria)

4.Methodology, learning tasks, syllabus and resources

4.1.Methodological overview

The course contents are organized in two main sections (A and B), corresponding to the descriptors of the title of the course: A) *Simulation of Chemical Processes*, and B) *Optimization of Chemical Processes*. The sequential order of the sections is important since *Optimization* is strongly based on models, which are actually resulting from the *Simulation* units or the whole flowsheet.

Both sections are divided into topics that group knowledge with a common leitmotiv. This way of distributing contents in compartments (i.e. topics) leads to a heterogeneous distribution of the topics (regarding their length), favouring topics with a higher or lower number of lectures. Something similar happens regarding the distribution of the types of lectures: some topics contain more theoretical issues while others almost lack them, but on the contrary require a stronger effort in the solving of practical cases (i.e. problems).

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Lectures and practice sessions devoted to problem-solving alternate along the course due to its strong practical character. Its spirit can be summarized in a sentence attributed to Confucius: "*I hear and I forget. I see and I remember. I do and I understand*".

In parallel with the lectures, there are scheduled several laboratory sessions with two main goals: approach the students to the use of commercial process simulation packages (*Aspen Plus, Aspen Hysys, UniSim*) and provide them with a practical experience to solve different kind of problems related to modelling in the process industry, which should be solved with the available and most suitable tools to the problem and its circumstances. These practice sessions are carried out in the *Laboratory of Process Simulation*. Similarly, other practice sessions (seminars) will deal with calculus tools (Spreadsheets, Matlab, EES, Phyton,...) which are extremely useful in order to solve the problems that are proposed in class.

4.2.Learning tasks

The course includes the following learning tasks:

- Lectures (**30 hours**). The theoretical aspects of the different topics will be provided. These sessions will be the scenario for proposing "model" problems related to the theoretical aspects shown in class.
- Practice sessions (**20 hours**). In these sessions the lecturer will solve problems and case studies previously offered to the students to be worked on their own. Likewise, students will be encouraged to take part in the solving process, proposing alternatives and/or doubts that have arisen along the autonomous solving process. These problems or case studies will be related to the theoretical aspects explained in lectures.
- Laboratory sessions (**8 hours**). The students will reinforce their theoretical knowledge by "doing". These sessions will always be *practical* seminars.
- Special sessions (**2 hours**). These will be complementary activities devoted to visits to industries, experts' talks, thematic seminars, etc.
- Guided projects (**14 hours**). Individual or group work in which 2 or 3 activities will be proposed along the course that will be supervised by lecturers.
- Project (**30 hours**). In groups of 2 or 3 people, students will solve a big scale problem. It will be supervised by lecturers and will count for the final mark.
- Study (**40 hours**). It is strongly recommended that students follow a study schedule from the very beginning until the end of the course.
- Assessment (**6 hours**). During the course several evaluation activities will take place as well as a final global exam to assess the achievements of the student as much in theory as in practice.

4.3.Syllabus

The course will address the following topics:

SECTION A. SIMULATION

- **Topic 1.** Simulation Concepts. Introduction: Models and Systems. Process Analysis. Commercial process simulation packages vs. "*ad-hoc*" tools. Software for simulation: process simulators, programming languages. Compilers and interpreters. Simulation and Optimization in Process Engineering.
- **Topic 2.** Diagrams, representations and simulation techniques. Block diagrams (BD), Flowsheet diagrams (PFD) and Pipe and Instrumentation Diagrams (P&ID). Recirculation, purge and bypass. Process Simulation techniques. Ordering and solving strategies. Degree of freedom analysis.
- **Topic 3.** Flowsheet diagram analysis. Resolution strategies. Flowsheet diagrams decomposition. Tear streams. Algorithm of *Sargent and Westerberg*. Algorithm of *Upadhye and Grens*. Numerical convergence techniques: Algorithms of *Newton* and *Wegstein*.
- **Topic 4.** Models for property prediction of chemicals. Models for thermodynamic properties estimation: Equations of State (EOS), Real vs. ideal mixtures. Activity models. Fugacity models. Partial pressure model, Enthalpy models, other properties (viscosity, Cp, ...).

- **Topic 5.** Models for auxiliary units. Conventions. Models for units operating in stationary mode: Mixers, Stream splitters, Component splitters. Impulsion equipment: Pumps, compressors, expanders.
- **Topic 6.** Models for conceptual reactors. Fixed conversion reactors: Relative stoichiometric coefficient matrix, Characteristic component for a given reaction. Equilibrium Reactors. Yield Reactors, Gibbs reactor.
- **Topic 7.** Models for ideal reactors: Plug flow reactor (PFR), Continuously Stirred Tank Reactor (CSTR), Batch Reactor (BATCH), Non ideal reactors.
- **Topic 8.** Separation Units I. Liquid-Vapour equilibrium. Phase splitters (flash). Characteristic operation conditions. Difference between state variables and operation variables in process streams.
- **Topic 9.** Separation Units II. Distillation and Rectification: Heuristic models for multicomponent distillation. Semi-rigorous models. Key issues for understanding rigorous models. Absorption and Stripping: Heuristic models.
- **Topic 10.** Models of units with heat exchange. Process units with heat exchange: Heat exchangers (HX) and reactors (R). With or without phase change. Entalphy balances. Effect of pressure.
- **Topic 11.** Simulation of units and processes in transient mode. Dynamic simulation of process units. Numerical techniques for calculation in dynamic mode. Case studies.
- **Topic 12.** Introduction to cost estimation of process units. Profitability and Benefit. Equipment amortization. Heuristic rules for process equipment dimensioning. Scale index. Williams rule. Simplified *Guthrie* method. Chemical industry economical indicators: CEPCI, Marshall&Swift and others.

SECTION B. OPTIMIZATION OF CHEMICAL PROCESSES

- **Topic 13.** Introduction to process optimization techniques and classification. Introduction to optimization of chemical processes. Elements required for optimization of chemical processes. Classification of Optimization techniques depending on their goals.
- **Topic 14.** Non-linear programming. Non-linear optimization (NLP) with or without restrictions. Powell method. Nelder y Mead method. Steepest descent methods. Commercial tools for optimization: EXCEL, Lingo and GAMS.
- **Topic 15.** Linear programming. Linear optimization (LP). Graphic resolution method. Linear SIMPLEX method. Restriction relaxation. SIMPLEX Matrix, Slack and Surplus variables, Basic and non-basic variables. Incoming variable and out coming variables selection criteria.
- **Topic 16.** Advanced optimization of chemical processes. Advanced optimization techniques for units and processes. Evolutive methods: Genetic algorithms, Simulated annealing, Evolutive methods, Tabu search.
- **Topic 17.** Optimization of heat exchanger networks (HENS). Introduction. Concept of energy integration. First and second principle of thermodynamics. Hot streams and cold streams. Hot service and cold service streams (duties). Minimum temperature increment. Cascade diagram. Composite curve and grand composite curve. Pinch temperature. Number of loops. Minimal energy consumption. Minimal number of HX.
- **Topic 18.** Dynamic optimization of process units.

4.4.Course planning and calendar

Further information concerning the timetable, classroom, office hours, assessment dates and other details regarding this course, will be provided on the first day of class or please refer to the EINA website (*http://eina.unizar.es*).

4.5.Bibliography and recommended resources