66212 - Simulation and Optimization of Chemical Processes

Información del Plan Docente

Academic Year	2016/17
Academic center	110 - Escuela de Ingeniería y Arquitectura
Degree	531 - Master's in Chemical Engineering
ECTS	6.0
Course	1
Period	First semester
Subject Type	Compulsory
Module	---

1.Basic info

1.1.Recommendations to take this course

1.2.Activities and key dates for the course

2.Initiation

2.1.Learning outcomes that define the subject

2.2.Introduction

3.Context and competences

3.1.Goals

3.2.Context and meaning of the subject in the degree

3.3.Competences

3.4.Importance of learning outcomes

4.Evaluation

5.Activities and resources

5.1.General methodological presentation

The learning process that has been planified for this subject is based on the following issues:

The themes of the subject are distributed in two well stablished blocks (A and B), corresponding to the descriptors of the title of the subject: A) *Simulation of Chemical Processes* , and B) *Optimization of Chemical Processes* . The sequence of blocks is important since *Optimization* if strongly based on models, which actually are resulting from the *Simulation* units or the whole flowsheet.

Both blocks are divided into themes that group knowledge with a common leitmotiv. This way of distributing matters in compartments (i.e. themes) leads to an inhomogeneous distribution of themes (regarding their lengths), favouring themes with a higher number of expositive sessions and other with lower. Something similar happens respecting the distribution of the types of lectures: some themes contain more theoretical issues while others are almost devoid of them, but on the contrary require a stronger effort in the resolution of practical cases (i.e. problems).

Theoretical lectures and practical sessions devoted to problem resolution are alternating along the course on demand. The subject has a 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 theoretical lectures (" *blackboard lectures* ") it has been planned several laboratory sessions with two main goals: approach the students to using commercial process simulation packages (*Aspen Plus, Aspen Hysys, UniSim*) and provide them with a hands-on experience to solve different kind of problems related to modelling in the process industry, that should be solved with the tools available provided that they adequate to the problem and the circumstances. These practical sessions are carried out in the Laboratory of Process Simulation. On the same way, several practical sessions will be provided on training with calculus tools (Spreadsheets, Matlab, EES, Phyton,...) which are extremely useful in order to solve the problems that are proposed in class.

5.2.Learning activities

The program offered to the student to assist him in achieving the foreseen results, implies the following activities:

Lectures (**30 h**) where the theoretical aspects of the different themes will be provided. Also these sessions will be the scenario for proposing "model" problems related to the theoretical aspects shown in class.

Problems and case studies solving sessions (20 h). 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 invited 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 exposed in the previously mentioned lectures.

Laboratory sessions (**8 h**). The student will reinforce its knowledge developed in lectures by "doing". These sessions will always be " *hands-on* " seminars.

Special sessions (**2 h**). These will be devoted to visits to industries, experts' talks, thematic seminars, etc... as a compliment to the previous formative activities.

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Tutored projects (**14 h** - *unattended* -) Conceived for personal work or in group. 2 or 3 activities will be proposed along the course that will be supervised by lecturers.

Big scale applied project (30 h). These consist of resolution by groups of students (2 or 3 per group) of a big scale problem with a limited although not null number of degrees of freedom. This work will be supervised by lecturers and will count for the final mark.

Personal study time (**40** h - *unattended* -). It is strongly recommended that the student follow a personal study schedule from the very beginning and that it extends up to the end of the course.

Evaluation (6 h). Partial evaluations and a final global exam will be carried out where it will be evaluated the achievements of the student as much in theory as in practice.

5.3.Program

The syllabus foreseen for the subject is the following:

BLOCK A.- SIMULATION

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.

2 Diagrams, representations and simulation techniques. Block diagrams (BD), Flowsheet diagrams (PFD) and Pipe and Instrumentation Diagram (P&ID). Recirculation, purge and bypass. Process Simulation techniques. Ordering and solving strategies. Degree of freedom analysis.

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-Raphson* and *Wegstein* .

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 (vistosity, Cp, ...).

5 Simple models for auxiliary units. Models for auxiliary units. Conventions. Models for units operating in stationary mode: Mixers, Stream splitters, Component splitters. Impulsion equipment: Pumps, compressors, expanders.

6 Models for conceptual reactors. Models for conceptual reactors. Fixed conversion reactors: Relative stoichiometric coefficient matrix, Characteristic compound for a given reaction. Equilibrium Reactors. Yield Reactors, Gibbs reactor.

7 Models for ideal reactors. Models for ideal reactors: Plug flow reactor (PFR), Continuously Stirred Tank Reactor

(CSTR), Batch Reactor (BATCH), Non ideal reactors.

8 Separation Units I. Liquid-Vapour equilibrium. Phase splitters (flash). Characteristic operation conditions. Difference between state variables and operation variables in process streams.

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.

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.

11 Simulation of units and processes in transient mode. Dynamic simulation of process units. Numerical techniques for calculation in dynamic mode. Case studies.

12 Introduction to cost estimation of process units. Introduction to cost estimation of chemical processes. 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.

BLOCK B.- OPTIMIZATION OF CHEMICAL PROCESSES

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 the goal.

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.

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.

16 Advanced optimization of chemical processes. Advanced optimization techniques for units and processes. Evolutive methods: Genetic algorithms, Simulated annealing, Tabu search. Case studies: application to reaction kinetics.

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 (PINCH). Number of loops. Minimal energy consumption. Minimal number of HX.

18 Dynamic optimization of process units.

5.4.Planning and scheduling

Calendar of lectures and Project deadlines

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The detailed calendar of activities, as well as the place where they will be celebrated is under the responsibility of the Engineering and Architecture School (EINA), and could be consulted in its web site (http://eina.unizar.es) on dates prior to the beginning of the new course. Additionally, every lecturer will inform about his/her availability for personal tutoring and possible modifications that can arise along the course.

5.5.Bibliography and recomended resources

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BB	Biegler, L.T.. Systematic methods of chemical process design / L.T. Biegler, I. E. Grossmann, and A.W. Westerberg Upper Saddle River : Prentice Hall, cop. 1997
BB	Douglas, James M.. Conceptual design of chemical processes / James M. Douglas New York [etc.] : McGraw-Hill, cop. 1988
BB	Edgar, Thomas F.. Optimization of chemical processes / Thomas F. Edgar, David M. Himmelblau, Leon S. Lasdon . - 2nd ed. Boston [etc.] : McGraw-Hill, 2001
BB	Jana, Amiya K.. Chemical process modelling and computer simulation / Amiya K. Jana . - 2nd ed. New Deli : PHI Learning, cop. 2011
BC	Cutlip, Michael B.. Resolución de problemas en ingeniería química y bioquímica con POLYMATH, Excel, y MATLAB / Michael B. Cutlip, Mordechai Shacham ; traducción, Ángel-Manuel Montaña Pedrero, Consuelo Batalla García . - 2ª ed. Madrid [etc.] : Pearson Educación, 2008
BC	Dimian, Alexandre C.. Integrated design and simulation of chemical processes / Alexandre C. Dimian . - 1st ed. Amsterdam : Elsevier, 2003
BC	Estrategias de modelado, simulación y optimización de procesos químicos / Luis Puigjaner ... [et al.] Madrid : Síntesis, D.L. 2006
BC	Knopf, F.C . Modeling, Analysis and Optimization of Process and Energy Systems / Knopf, F.C. John Wiley and Sons, New Jersey. 2012.
BC	Mathematical modeling in chemical engineering / Anders Rasmuson ... [et.al.] Cambridge (United Kingdom) : Cambridge University Press, cop. 2014
BC	Nauman, E. Bruce. Chemical reactor design, optimization, and scaleup / E. Bruce Nauman . - 2nd ed. Hoboken (New Jersey) : John Wiley & Sons, cop. 2008

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BC	Seider, Warren D.. Process design principles : synthesis, analysis, and evaluation / Warren D. Seider, J.D. Seader, Daniel R. Lewin New York [etc.] : John Wiley, 1999