Course guide
820542 - PSCPQ - Planning and Scehduling of Chemical Processes

Last modified: 27/05/2024

Unit in charge: Barcelona East School of Engineering
Teaching unit: 713 - EQ - Department of Chemical Engineering.

Degree: BACHELOR'S DEGREE IN CHEMICAL ENGINEERING (Syllabus 2009). (Optional subject).

Academic year: 2024 **ECTS Credits:** 6.0 **Languages:** Catalan, English

LECTURER

Coordinating lecturer: MOISES GRAELLS SOBRE

Others: Segon quadrimestre:
MOISES GRAELLS SOBRE - T10
ANA SOMOZA TORNOS - T10

DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES

Specific:
3. Analyse, design, simulate and optimise processes and products.
4. Design, manage and run simulation, control and instrumentation procedures in chemical processes.

Transversal:
1. SUSTAINABILITY AND SOCIAL COMMITMENT - Level 3. Taking social, economic and environmental factors into account in the application of solutions. Undertaking projects that tie in with human development and sustainability.
6. THIRD LANGUAGE. Learning a third language, preferably English, to a degree of oral and written fluency that fits in with the future needs of the graduates of each course.

TEACHING METHODOLOGY

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LEARNING OBJECTIVES OF THE SUBJECT

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STUDY LOAD

Type	Hours	Percentage
Self study	90,0	60.00
Hours large group	45,0	30.00
Hours small group	15,0	10.00

Total learning time: 150 h

CONTENTS

(ENG) -

Description:
(ENG) 1. Introduction to Modelling and Optimization (2h). Decision-making and tools: modelling, simulation, optimization. Definitions: Model, variable, parameters, constraints and objective function. Model limitations and model levels. Optimality and sub-optimal results. Divide and conquer. Computing time as a problem variable. Preliminary calculations: estimating, bounding and heuristics. Exercises.
2. Introduction to Process Planning and Scheduling (2h). Process flexibility and resource allocation. The Design-Operation Paradigm. Time independent problems and time dependent problems: continuous processes, semi-continuous processes and batch processes. Short-term decisions and long-term decisions. Reactive scheduling. Information flow through levels and models. Review exercises.
3. Continuous Processes (4h). Blending and flowsheeting problems. Introduction to linear programming (LP) and optimization: graphical interpretation. Importance of constraints. Problem definition. Modelling and solving with MS-Excel (Solver). Optimization tools: LP sensitivity analysis. Exercises using EXCEL (Blending.xls, Refynery.xls, Alkyl.xls).
4. Semi-Continuous processes (4h). Standard problems: the transportation problem. Formulation and solution using Solver. Semi-continuous processes: parallel production lines (extruders, fed-batch reactors, etc.). Assignment of time to lines. Model limitations (changeovers and sequencing, etc.). Study and discussion of possible objective functions. Analysis and decision-making. Exercises using EXCEL (Transport.xls, Production_lines.xls, Solver_tester.xls).
5. Assignment problems (4h). Introduction to GAMS. Solving the transport and the parallel lines problems using GAMS. Comparing GAMS and the Excel Solver. Standard problems: the knapsack problem. Introduction to integer programming (MIP). Exercises using GAMS (Trnsport.gms, knpsk.gms).
6. Sequencing problems I (4h). Introduction to set-up and cleaning needs. Constant and sequence dependent changeover times. The changeover matrix. Simulation using EXCEL.
7. Dynamic processes (4h). A first-order kinetics model. Ordinary Differential Equations using Excel (Euler Method). Optimization of the operation of a batch reactor. Objective function: introduction to cyclic operations, idle time and cycle time. Maximum operation performance. Maintenance planning. Exercises using Excel (Maintenance.xls).
8. Introduction to discontinuous processes (4h). Need for the batch-wise operation mode: batch chemical process industries. Concepts and definitions: batch size, cycle time and size factor. Debottlenecking: identification of time and size limiting stages. The Gantt chart. Detail of the model and granularity. Exercises and preliminary hand calculations.

Full-or-part-time: 50h
Theory classes: 10h
Laboratory classes: 10h
Self study : 30h

(ENG) -

Description:
(ENG) 11. Storage. Storage needs for adjusting production sub-trains: matching continuous and batch processes. Storage policies in batch processing: ZW, FW, UIS, FIS. Storage location and sizing. The Lowest Storage Level Rule (LSL). Exercises using Excel (Roblon.xls, B&B.xls) and GAMS (batchdes.gms).

12. Sequencing problems II (4h). The Travelling Salesman Problem (TSP). Problem formulation. Limitation of the solution time, decision making and need for sub-optimal solutions. Greedy heuristics. Metaheuristics and stochastic methods. Developing and programming algorithms: the MSES method. Exercises using Excel (TSP.xls).

13. Scheduling of batch processes I (4h). Elementary formulations for the multiproduct case. Basic sequencing and assignment variables. Binary variables and problem size. Time discretization. Enhanced formulations: time slots, the State Task Network (STN). Formulation exercises using GAMS.

14. Scheduling of batch processes II (4h). Advanced model development. Representing logical constraints: from Big-M to disjunctive programming. Enhanced formulations and tricks: introducing cuts, tightening relaxations, breaking symmetry, tuning parameters, etc. Formulation exercises using GAMS.

15. Detailed scheduling of batch chemical processes (8h). Review of available commercial software: BatchPlus (AspenTech), SuperPro & SchedulePro (Intelligen Inc.), etc. Recipe management standards: the ISA88. Development of a case study simulation and debottlenecking problem in the biotechnological or pharmaceutical industry.

Full-or-part-time: 50h
Theory classes: 10h
Laboratory classes: 10h
Self study : 30h

(ENG) TEMES 11-15

Full-or-part-time: 50h
Theory classes: 10h
Laboratory classes: 10h
Self study : 30h

GRADING SYSTEM

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BIBLIOGRAPHY

Basic:
- Edgar, Thomas F.; Himmelblau, David Mautner; Lasdon, Leon S. Optimization of chemical processes. 2nd ed. Boston [etc.]: McGraw-Hill, cop. 2001. ISBN 0070393591.
- Biegler, Lorenz T.; Grossmann, Ignacio E.; Westerberg, Arthur W. Systematic methods of chemical process design. Upper Saddle River (New Jersey): Prentice Hall PTR, cop. 1997. ISBN 0134924223.
- Mah, Richard S. H. Chemical process structures and information flows. Boston [Mass.] [etc.]: Butterworths, cop. 1990. ISBN 0750692308.