320069 - SOCPQ - Simulation, Optimization and Control of Chemical Processes

Coordinating unit: 205 - ESEIAAT - Terrassa School of Industrial, Aerospace and Audiovisual Engineering
Teaching unit: 713 - EQ - Department of Chemical Engineering
Academic year: 2019
Degree: BACHELOR'S DEGREE IN CHEMICAL ENGINEERING (Syllabus 2009). (Teaching unit Compulsory)
ECTS credits: 6  
Teaching languages: Catalan

Teaching staff
Coordinator: Antoni Escalas Cañellas
Others: Antoni Escalas Cañellas
Josep Maria Guadayol Cunill
Jorge Macanás de Benito

Prior skills
The lecturers of this subject consider essential for the students to be able to follow this course properly: To have previously passed the subjects of Fundamentals of chemical engineering (Q4) and Industrial control and automation (Q4), as well as having completed the courses of Basic operations 1 (Q5), Chemical Reaction Engineering (Q5) and being enrolled in the course Basic Operations 2 (Q6).

Degree competences to which the subject contributes

Specific:
- CE20. CHE: ability to analyse, design, simulate and optimise processes and products.
- CE22. CHE: Ability to design, manage and operate procedures for the simulation, control and instrumentation of chemical processes.
- CE19. CHE: Knowledge of material and energy balances, biotechnology, the transfer of materials, separation operations, chemical reaction engineering, the design of reactors, and the reuse and transformation of raw materials and energy resources.

Transversal:
- 07 AAT N3. SELF-DIRECTED LEARNING - Level 3. Applying the knowledge gained in completing a task according to its relevance and importance. Deciding how to carry out a task, the amount of time to be devoted to it and the most suitable information sources.
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Teaching methodology

- Presentation classroom sessions by the lecturer.
- Application classroom sessions, practical work in the classroom
- Practical laboratory sessions.
- Autonomous study and exercises.
- Completion of an independent project simulation DWSIM.

In presentation sessions the lecturer expands the theoretical basis of the material already seen in "Industrial Control and Automation", focusing on applications in chemical processes. We also introduce the concepts and methods of simulation and process optimization illustrating them with examples appropriate to facilitate understanding.

Practical sessions in the classroom will be of two kinds:
a) sessions in which the lecturer guides students to analyze data and solve problems by applying techniques, concepts and theoretical results.
b) examination sessions and/or presentation of work.

The sessions will include practical laboratory work:
Simulation lab sessions where design and optimisation chemical processes will be performed through the simulation software.

Simulation project - Self-directed learning
Each couple of students will be assigned an individual project simulation of chemical processes with DWSIM, to be developed independently throughout the semester. This project will be developed primarily outside of the classroom, though 2-3 laboratory sessions (mostly during the 2nd bimester) will be devoted to student work on the project, supervised by the lecturer.

Learning objectives of the subject

- To familiarise students with the techniques of prediction and estimation and data optimization techniques.
- To develop the student's ability to apply these techniques wisely.
- To introduce students to the techniques of control chemical processes themselves.
- To introduce students to different commercial softwares to simulate the chemical processes from the design stage to the control and optimization.
- To develop specific skills associated with academic and transverse detailed below.
  Specific skills:
  - Ability to design, manage and operate procedures for simulation, control and instrumentation for chemical processes.
  - Ability to implement process optimization and chemicals.
  - Knowledge and application of the terminology used to describe the concepts relevant to this matter.

Generic skills:
- Ability to formulate and solve problems
- Critical reasoning
- Autonomous learning
- Ability to work in group
- Time management and organization of work
- Ability to write and develop projects
## Study load

<table>
<thead>
<tr>
<th>Study load</th>
<th>Hours large group:</th>
<th>Hours medium group:</th>
<th>Hours small group:</th>
<th>Guided activities:</th>
<th>Self study:</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Total learning time:</strong> 150h</td>
<td>30h</td>
<td>15h</td>
<td>15h</td>
<td>6h</td>
<td>84h</td>
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<tr>
<td></td>
<td>20.00%</td>
<td>10.00%</td>
<td>10.00%</td>
<td>4.00%</td>
<td>56.00%</td>
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</tbody>
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### Content

<table>
<thead>
<tr>
<th>T1. INDUSTRIAL CONTROL APPLIED TO CHEMICAL PROCESSES</th>
<th>Learning time: 75h</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Theory classes: 30h</td>
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<tr>
<td></td>
<td>Self study: 45h</td>
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</tbody>
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**Description:**
Application of control to chemical engineering processes and their various operations.

- **CONTINUOUS CONTROL**
  - Feedback control.
  - Feedforward control.
  - Feedforward-feedback control.
  - Relation control.
  - Cascade control.
  - Auctioneering control.
  - Inferential control.
  - Optimisation of control systems.

- **DISCRETE CONTROL**

**Specific objectives:**
- The ability to apply the control techniques covered in this subject to chemical processes.
- An understanding of feedforward systems.
- An understanding of control systems based on examples.
- The ability to optimise control systems.
## T2. PROCESS SIMULATION

<table>
<thead>
<tr>
<th>Learning time: 51h</th>
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<tbody>
<tr>
<td>Theory classes: 0h</td>
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<tr>
<td>Practical classes: 10h</td>
</tr>
<tr>
<td>Laboratory classes: 10h</td>
</tr>
<tr>
<td>Self study: 31h</td>
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</tbody>
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### Description:
- Prediction of physical and chemical properties in single-component systems.
- Equations of state.
- Multicomponent prediction of physicochemical properties in one-component systems.
- State equations.
- Multicomponent systems.
- Prediction of thermodynamic properties.
- Application of predictive models in DWSIM.
- Design of unit operations in DWSIM
- Design of a process in DWSIM
- Design of process control in DWSIM
- Other simulation programs

### Related activities:
- Introduction to DWSIM simulation software, and development of real processes and operations.
- Simulation laboratory practices
- Development of an individual project

### Specific objectives:
- To learn the basics of predictive models used in simulation programs on the market.
- To know how to interpret the validity of the available data according to their origin.
- To relate the different physicochemical and thermodynamic properties.
- To estimate the value of properties not available.
- To work with the DWSIM software.
- To provide an overview of the possibilities of process simulation as a tool for computer systems analysis, which minimizes risks and costs in experimentation.
T3. PROCESS OPTIMISATION

**Learning time:** 24h
- Theory classes: 0h
- Practical classes: 5h
- Laboratory classes: 5h
- Self study: 14h

**Description:**
- Introduction to Optimisation. Optimisation in Chemical Engineering
- Theory and optimisation algorithms: Constrained/Unconstrained Optimisation
- Linear / nonlinear problems
- Linear programming, simplex method, nonlinear programming
- Process simulation and its link to optimisation.

**Related activities:**
- Application of the DWSIM simulation software, and other, to the optimisation of real processes and operations.

**Specific objectives:**
- Developing the ability to recognise and solve situations requiring the use of optimisation tools.
- Obtaining knowledge on mathematical optimisation algorithms and their application
- Using computer optimisation tools.
- Offer a range of optimization techniques able to solve many problems that can arise in Chemical Engineering.

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**Qualification system**

Oral and written tests 75%:
- 1st bimester exam (weight: 37%). Within the exam, 2/3 of the weight correspond to Control/Automation, with the other 1/3 is for Simulation.
- 2nd bimester exam (weight 38%). Within the exam, 2/3 of the weight correspond to Control/Automation, with the other is for 1/3 for Simulation.

Laboratory: 5%

Other deliveries (Simulation Project): 20%

Note: The Simulation project also serves as an evaluation tool for the Autonomous Learning skill.

Make-up exam ("Reconducció"): The students who obtain a grade less than 5.0 in the 1st bimonthly exam will be allowed to conduct a make-up exam ("reconducció") on the same day and within the same timetable established by the school for the final exam. Those interested in doing the make-up exam will communicate it to the coordinator in advance, through the means established by the coordinator and within specified the deadline.
**Bibliography**

**Basic:**


**Complementary:**


