PERSONA CIÈNCIA EMPRESA
UNIVERSITAT RAMON LLULL

COURSE: COMPUTER SCIENCE AND NUMERICAL CALCULUS

SUBJECT MATTER: Computer Sciences and Numerical Calculus
MODULE: Basic Formation
PROGRAM: Degree in Chemical Engineering

GENERAL FEATURES

Type: ☑ Basic Formation, ☐ Compulsory, ☐ Elective
☐ Final Degree Project, ☐ Internship
Duration: Annual **Semester/s**: 1 y 2
Number of ECTS Credits: 6
Language/s: Spanish, Catalan

DESCRIPTION

SHORT DESCRIPTION AND JUSTIFICATION

Computers are an essential part of our daily life and of the professional activities of a chemical engineer (reporting, presentations, project development, data capture and processing, resource management, documentation…)

This course aims to present the use of computers and computing techniques for its use in science. These skills are fundamental both for next courses in the program and for the forthcoming professional work of the graduates.

The course includes as its essential contents an introduction to hardware and software, the use of GUI-based operating system, use of a spreadsheet program for solving scientific and engineering problems, algorithms, structured programming, and the description and use of some basic numerical methods.

COMPETENCES

- Be able to understand and apply basic knowledge of computer science (office applications, algorithms, programming and numerical methods) that, grounding from knowledge acquired in general secondary education, are needed for the practice of chemical engineering. (→E1, CB1)
- Be able to identify, formulate and solve basic problems in chemistry and engineering by making use of numerical and computational methods. (→E7, CB2)
- Be able to convey information, ideas, problems and solutions to both specialized and non-specialized audiences. (→CB4)
- Be knowledgeable about use and programming of computers, operating systems, databases and software with engineering applications. (→FB3)

PREREQUISITES

According to the program planning and academic regulations.

CONTENTS

1. Introduction to information systems
   Hardware. Software
2. Introduction to operating systems and use of a GUI-based operating system
   Use of a graphical user interface. Files and documents management. Operating system settings management.
3. Use of a spreadsheet application
   Entering text, numbers and formulas. Use of mathematical, logical, text, search and reference functions. Use of formatting and conditional formatting.
4. Algorithms
   Definition. Algorithms representation. Control structures: sequence, selection and repetition. Variables and data types. Modularization.
5. Structured programming
   Introduction to Visual Basic. Visual Basic for Applications programming.
6. Use of a database application
   Database design: fields, tables, indices and relations. Building queries to exploit the database.
7. Interpolation
   Linear interpolation. Polynomial interpolation. Interpolation error.
8. Numerical differentiation
   Finite increments. Differentiation based on interpolation polynomials. Methods based on central differences.
9. Numerical integration
   Elementary methods. Trapezoidal rule.
10. Root finding
    Root localization and bounding. Bisection methods. Tangent, secant and modified Newton methods.
11. Empirical equations fitting
    Polynomial fit. Linearization. Least squares method.

METHODOLOGY

LEARNING ACTIVITIES

Learning Activities	Hours	ECTS Credits	Competences
Lectures	35	1,3	E1, CB1, FB3
Case and Problem-Solving Sessions	27	1,0	E1, CB1, E7, CB2, FB3
Seminars	-	-	-
Practical & Lab Work	22	0,8	E1, CB1, E7, CB2, FB3
Oral Presentations	3	0,1	E7, CB2, CB4, FB3
Personal Study	54	2,0	E1, CB1, E7, CB2, FB3
Assessment Tasks (Exams, Continuous Assessment…)	22	0,8	E1, CB1, E7, CB2, FB3
TOTAL	**162**	**6**	

TEACHING METHODOLOGY

The teaching methodology used in the course relies on the availability of computers by the students. Most of the face-to-face sessions combine part of lecturing and part of practical work. This produces four different types of interactions in the classroom: expositions (content presentation), demonstrations (the instructor shows some tasks are done, or some problems are solved, and the learners follows replicating the actions on their own computer), active moments (the learners solve a problem which is later-on solved by the instructor), and autonomous work (the learners work on their pending tasks and get personal advise as needed). In this way, the learners take an active role, facilitating the acquisition of knowledge and the practice in solving problems.

The course has two blocks of practice tasks, done in groups of 2 or 3 people. In these practices, the students are asked to solve a problem proposed by the teaching team. Then, they are asked to present and defend their work.

For the personal study, software, problem sets, on-line assessment tests, documents from the face-to-face sessions and bibliographic resources are provided.

ASSESSMENT

ASSESSMENT METHODS

Assessment Methods	Weight	Competences
Final Exam	25%	E1, CB1, E7, CB2, FB3
Midterm Exam/s	25%	E1, CB1, E7, CB2, FB3
Continuous Assessment Activities	-	
Reports and Presentations	25%	E7, CB2, CB4, FB3
Lab or Field Work	25%	E7, CB2, FB3
Projects	-	
Host Student Evaluation	-	
Participation	-	

LEARNING OUTCOMES

- Students must be knowledgeable about fundamental algorithmic structures and basic programming, making algorithms according to some prerequisites, analyzing already made algorithms, and correcting them if needed. (→ E1, CB1, FB3)
- Students must be knowledgeable about basic algorithms and tools of numerical methods, selecting and justifying the most appropriate methods to do approximate calculations to estimate the error in these calculations. (→ E1, CB1, FB3)
- Students must be able to elaborate spreadsheet templates and simple programs to carry out systematic calculations and/or to solve problems in chemical engineering. (→ E7, CB2, FB3)
- Students must be able to properly use numerical methods tools to solve problems in chemistry, biosciences and chemical engineering. (→ E7, CB2, FB3)
- Student must be able to document their spreadsheet templates and their computer programs. (→ CB4)

QUALIFICATION

The course assessment considers the grades of the practices (PR), the continuous assessment tasks (EC), the partial exams (EP), the final exam, either in first or second examination period, (EF) and extra credit activities (BN). All the grades are out of 10 and are maxed to 10.

A grade for the practical work (NP) is obtained as a average of the practices and the continuous assessment: NP = (PR + EC)/2, where both the practice grade (PR) and the continuous assessment grade (EC) are weighted averages of the different tasks. The grade for the practical work must be equal or over 4 to pass the course. A retaken grade for the practical work can be obtained by making remedial practice tasks, before any final exam of the course. This retake must be asked in advance to the final exam and will be maxed to 5.

A grade for the exams (NE) is obtained assessing independently both parts of the course, one per semester. The grade, which must be equal or over 4, is calculated taking the minimum of the grades obtained for both semesters: NE = min(max(EP1; 2·EF1P); max(EP2; 2·EF2P)) where EPx relates to the corresponding partial exams and EFxP to the corresponding part in the final exam (out of 5).

If either the grade for the practical work or the grade for the exams were below 4, the final grade would be the minimum of both grades.

If both the grade for the practical work (NP) and the grade for the exams (NE) are equal or over 4, then the final grade (CF) of the course, either in first or second examination period, is determined according to the following expression:

$$CF = 0{,}5\ NP + 0{,}25\ EP + 0{,}25\ EF$$

Alternatively, the final grade can be obtained as

$$CF = 0{,}5\ NP + 0{,}5\ (\max(EP1; 2\cdot EF1P) + \max(EP2; 2\cdot EF2P))/2$$

In any case, both the grade for the practical work (NP) and the grade for the exams (NE) must be equal or over 4. The final grade will correspond to the option that delivers the largest grade.

If and only if this grade is equal or over 5, the student passes the course and the final grade is augmented with a 10% of the extra credit grade (BN): CF = CF + 0,1 BN. This extra credit grade can be obtained by doing optional tasks oriented towards improving the teaching and learning processes.

ASSESSMENT OF THE COMPETENCES

The competence E1/CB1 will be assessed through a function of the exam grades. To assess the competence E2/CB7 and FB3, the final grade of the course will be used. To assess the competence CB4, the grade for the practices is used.

BIBLIOGRAPHY

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- MICROSOFT. Office 2013 VBA Documentation. https://www.microsoft.com/en-us/download/details.aspx?id=40326
- JOYANES AGUILAR, L. Fundamentos generales de programación; McGrawHill; Madrid, 2012; ISBN: 978-607-15-0818-8
- WALKENBACH, JOHN; Excel VBA Programming for Dummies; John Wiley & Sons; 4th Revised edition (27 Oct. 2015); ISBN: 978-1119077398
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DOCUMENT HISTORY

PREVIOUS REVISIONS
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CURRENT REVISION
March 25th, 2019, Dr. Jordi Cuadros