UNIVERSIDAD DE CASTILLA - LA MANCHA

GUÍA DOCENTE

1. General information

Course: COMPUTER APPLICATIONS IN CHEMICAL ENGINEERING
Code: 57705
Type: BASIC
ECTS credits: 6
Degree: 344 - CHEMICAL ENGINEERING
Academic year: 2023-24
Center: 1 - FACULTY OF SCIENCE AND CHEMICAL TECHNOLOGY
Group(s): 21
Year: 1
Duration: C2
Main language: Spanish
Second language: English
Use of additional languages:
English Friendly: Y
Web site:
Bilingual: N

Lecturer: **JESUS MANUEL GARCIA VARGAS** - Group(s): **21**

Building/Office	Department	Phone number	Email	Office hours
Enrique Costa Novella	INGENIERÍA QUÍMICA	3502	JesusManuel.Garcia@uclm.es	monday, wednesday and thursday from 11.30 to 13.30

Lecturer: **JOSE LUIS VALVERDE PALOMINO** - Group(s): **21**

Building/Office	Department	Phone number	Email	Office hours
Enrique Costa. Despacho 11	INGENIERÍA QUÍMICA	926295300	joseluis.valverde@uclm.es	Monday, wednesday and thursday from 12 to 13h. It is recommended to send previously an email to check availability in order to avoid crowds.

2. Pre-Requisites

Not established

3. Justification in the curriculum, relation to other subjects and to the profession

Justification in the curriculum and relationship with the profession

This course introduces the future graduate in Chemical Engineering to computer tools that will be used profusely throughout his career and that, in many cases, their mastery is something distinctive of the profession of Chemical Engineering in terms of simulation, design, regulation and optimization of chemical processes. This would be the case of the commercial simulator ASPEN HYSYS.

It introduces the student into the use of Microsoft programs: VISIO, basic for the drawing and configuration of flow diagrams, and EXCEL, basic for the realization of all types of calculations and graphics that the student will need throughout his academic and professional life. The latter will be used together with the Visual Basic for EXCEL Applications (EXCEL-VBA) language to introduce the student to basic concepts of structured and modular programming that will be very useful in the development of advanced calculations in Chemical Engineering.

Finally, the student will be introduced into the use of the commercial simulator ASPEN HYSYS for the calculation of simple chemical processes, conceptually approachable by first year students.

Relation with other subjects

The EXCEL-VBA tool will be used in all the subjects of the GRADUATE. The VISIO tool will be used in all the project work of the subjects that involve studies of chemical processes, especially Projects.

The Aspen HYSYS simulator will be used essentially in the following subjects:

Second course:

Mass and Energy Balances

Fluid Mechanics

Heat Exchange

Thermotechnics

Third course:

Separation Operations

Chemical Reaction Engineering

Integrated Laboratory of Basic Operations and Chemical Reaction Engineering

Instrumentation and Control

Fourth course:

Projects

Integrated Laboratory of Processes and Products

Coal, Petroleum and Petrochemical Technology

Chemical and Energy Process Simulation

Simulation of Chemical and Environmental Processes

Renewable Energies and Energy Evaluation of Chemical Processes

Technology for the Decontamination and Purification of Gases

4. Degree competences achieved in this course

Course competences

Code	Description
E03	Basic knowledge about the use and programming of computers, operating systems, databases and computer programs with application in engineering.
G03	Knowledge in basic and technological subjects, which enables them to learn new methods and theories, and give them versatility to adapt to new situations.
G12	Proficiency in a second foreign language at level B1 of the Common European Framework of Reference for Languages
G13	Knowledge of Information and Communication Technologies (ICT).
G14	Proper oral and written communication
G16	Management capacity and information planning
G20	Ability to analyze and solve problems
G21	Ability to learn and work autonomously
G22	Ability to apply theoretical knowledge to practice
G23	Creativity and initiative

5. Objectives or Learning Outcomes

Course learning outcomes

Description

To understand the key objectives in the marketing subsystem.

To master the basic scientific terminology as well as the handling of units and their conversions.

To be able to program in the Visual Basic for Applications (VBA) language within the MS-Excel tool environment.

To know the Office tools of greatest interest for a Graduate in Chemical Engineering.

6. Units / Contents

Unit 1: INTRODUCTION TO EXCEL AND VISIO

Unit 1.1 Introduction to EXCEL. Basic concepts. Calculations and graphics. The SOLVER tool. Examples.

Unit 1.2 Macros in EXCEL. Examples.

Unit 1.3 Advanced concepts in EXCEL. Buttons, boxes, forms, controls and menus. Examples

Unit 1.4 Introduction to VISIO. Basic concepts. Forms. Block diagrams and information flow diagrams. Organizational charts. Examples

Unit 1.5 Use of VISIO in the construction of chemical process diagrams. Examples

Unit 2: SOLVING NUMERICAL PROBLEMS USING EXCEL

Unit 2.1 Basic numerical procedures. Matrix operations. Numerical resolution of linear equations. Interpolation. Numerical integration of functions and discrete data. Numerical differentiation. Calculation of the roots of functions of one variable and polynomials. Smoothing of experimental data. Linear regression. Examples

Unit 2.2 Advanced numerical procedures. Non-linear regression. Solving systems of nonlinear equations. Solving ordinary differential equations: Initial value problems. Solving differential equations: boundary value problems. boundary value problems. Examples

Unit 3: INTRODUCTION TO VISUAL BASIC PROGRAMMING FOR EXCEL APPLICATIONS (EXCEL-VBA) AND ITS USE IN CHEMICAL ENGINEERING PROBLEM SOLVING.

Unit 3.1 Fundamentals of programming in Visual Basic for EXCEL Applications. Introduction. Mechanics of code writing. Basic concepts of the code in VBA CODE. Data types, constants and variables. Arrays. Arithmetic and logical operations. Basic control structures and commands. Basic algorithms. Examples

Unit 3.2 Modular programming. General organization of VBA modules. Subroutines. Predefined functions in VBA. Examples.

Unit 3.3 Description of modules and their handling. Matrix operations and solving algebraic equations. algebraic equations. Interpolation and numerical extrapolation. Integration Numerical integration of functions. Evaluation of functions and derivatives. Differentiation and calculation of roots of functions. Modeling of experimental data. Solving of systems of nonlinear equations. Differential equations. Examples. Translated with www.DeepL.com/Translator (free version)

Unit 3.4 Solving Chemical Engineering problems. Fluid flow. Transmission of Heat. Matter transfer. Chemical Reaction Engineering. Control of Chemical Control of Chemical Processes. Examples.

Unit 4: INTRODUCTION TO THE USE OF HYSYS AS A SIMULATION TOOL FOR PROCESSES.

Unit 4.1 Introduction to the use of HYSYS. Thermodynamic packages. Components Hypothetical components. Degrees of freedom. Cases and examples.

Unit 4.2 Use of HYSYS in the simulation of simple chemical processes. Basic calculations. Mass and energy balances. Basic operations. Chemical reactors. Examples

7. Activities, Units/Modules and Methodology

Training Activity	Methodology	Related Competences (only degrees before RD 822/2021)	ECTS	Hours	As	Com	Description
Class Attendance (practical) [ON-	Work with simulators	G03 G12 G13 G16 G20	1.7	42.5	N	-	

SITE]		G21 G22 G23					
Other off-site activity [OFF-SITE]	Problem solving and exercises	G12 G13 G14 G16 G20 G21 G22 G23	3.6	90	Y	N	
Final test [ON-SITE]	Assessment tests	G13 G14 G16 G20 G21 G22 G23	0.1	2.5	Y	Y	
Workshops or seminars [ON-SITE]	Project/Problem Based Learning (PBL)	G12 G13 G16 G20 G21 G22 G23	0.1	2.5	N	-	
Class Attendance (theory) [ON-SITE]	Lectures	G12 G16 G20 G21 G22	0.5	12.5	N	-	
	Collaborative on line international learning (COIL)		6	150	Y	N	
		Total:	**12**	**300**			
		Total credits of in-class work: 2.4					**Total class time hours: 60**
		Total credits of out of class work: 3.6					**Total hours of out of class work: 90**

As: Assessable training activity
Com: Training activity of compulsory overcoming (It will be essential to overcome both continuous and non-continuous assessment).

8. Evaluation criteria and Grading System

Evaluation System	Continuous assessment	Non-continuous evaluation*	Description
Test	40.00%	40.00%	Examinations with practical questions. Four tests will be considered
Assessment of problem solving and/or case studies	60.00%	60.00%	Ms-Excel-VBA and Visio exercises resolution, numerical problems
Total:	**100.00%**	**100.00%**	

According to art. 4 of the UCLM Student Evaluation Regulations, it must be provided to students who cannot regularly attend face-to-face training activities the passing of the subject, having the right (art. 12.2) to be globally graded, in 2 annual calls per subject , an ordinary and an extraordinary one (evaluating 100% of the competences).

Evaluation criteria for the final exam:

Continuous assessment:

The evaluation of this course will require the completion of a series of activities:

1. Exams with practical questions on the contents taught in the course; four evaluative tests will be considered for each of the thematic units.
2. Resolution of Ms-Excel-VBA and Visio exercises (Thematic Unit 1).
3. Solving numerical problems manually and with the help of MS-Excel-VBA applications (Thematic Unit 2).
4. Solving programming problems in MS-Excel-VBA environment (Thematic unit 3).
5. Solving simulation problems of simple chemical processes: material and energy balances (thematic unit 4).

The course will be passed provided that in each of these activities a minimum grade of 4.0/10 is reached and an average value for all of them higher than 5.0/10.

If the course is not passed, a final exam will be considered that will cover all the aspects covered in the course. The course will be considered passed when the average grade is higher than 5.0/10.

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Non-continuous evaluation:

n the final test, activities will be proposed to evaluate competences related to Problem Solving or Case Studies.

Specifications for the resit/retake exam:

If the course is not passed, a final exam will be considered that will cover all the aspects covered in the course. The course will be considered passed when the average mark is higher than 5.0/10.

Specifications for the second resit / retake exam:

As it is a first year subject, it is understood, with the recently approved university regulations for students, which obliges the student who enrolls in a subject to use up all the exam dates even if he/she does not take any test, that it should not be affected by special exam dates such as the ones mentioned. In the remote case, if this were to occur, the regulations of the center or the university would be used to resolve this particularity.

9. Assignments, course calendar and important dates

Not related to the syllabus/contents

Hours	**hours**

Unit 1 (de 4): INTRODUCTION TO EXCEL AND VISIO

Activities	**Hours**
Class Attendance (practical) [PRESENCIAL][Work with simulators]	35

Comment: The calendar is approximate as it will depend on the beginning of the school year and holidays. This should be corrected administratively. They are taught one hour each day during the weeks of the course with the design approved by the Faculty Board.

Unit 2 (de 4): SOLVING NUMERICAL PROBLEMS USING EXCEL

Activities	**Hours**
Class Attendance (practical) [PRESENCIAL][Work with simulators]	20

Unit 3 (de 4): INTRODUCTION TO VISUAL BASIC PROGRAMMING FOR EXCEL APPLICATIONS (EXCEL-VBA) AND ITS USE IN CHEMICAL ENGINEERING PROBLEM SOLVING.

Activities	**Hours**
Class Attendance (practical) [PRESENCIAL][Work with simulators]	60

Unit 4 (de 4): INTRODUCTION TO THE USE OF HYSYS AS A SIMULATION TOOL FOR PROCESSES.

Activities	**Hours**

Class Attendance (practical) [PRESENCIAL][Work with simulators]	35

Global activity	
Activities	**hours**
Class Attendance (practical) [PRESENCIAL][Work with simulators]	150
Total horas:	150

10. Bibliography and Sources

Author(s)	Title/Link	Publishing house	Citv	ISBN	Year	Description
Cordero Barbero, Alicia	Cálculo Numérico : teoría y problemas	UPV		978-84-9705-539-0	2004	
Chapra, Steven C.	Métodos numéricos para ingenieros	McGraw-Hill		978-970-10-6114-5	2007	
FINLAYSON, Bruce A.	Nonlinear analysis in chemical engineering	McGraw-Hill		0-07-020915-4	1980	
Jacobson, Reed	Programación con Microsoft Excel versión 2000 : acros y Visu	McGraw-Hill		84-481-3248-3	2002	
Kincaid, David	Análisis numérico : las matemáticas del cálculo científico	Addison-Wesley Iberoamericana		0-201-60130-3	1994	
Riggs, James B.	An introduction to numerical methods for chemical engineers	Texas Tech University Press		0-89672-334-8	1994	
Seider, Warren D.	Process design principles : synthesis, analysis and evaluati	John Wiley and Sons		0-471-24321-4	1998	
Valverde, J.L.; Sánchez, M.L.; Jiménez, C.; Carmona, M.	Métodos numéricos y programación en EXCEL-VBA para ingenieros químicos	Editorial académica española	Saarbrüken, Alemania	978-3-659-08529-1	2014	
Walkenbach, John	Excel 2007 : programación con VBA	Anaya Multimedia		978-84-415-2298-5	2007	
	NUMERICAL recipes in Fortran 77 : The art of scientific com	Cambridge University Press		0-521-43064-X	1999	