

Degree programme	Type	Course
Chemistry	FB	1

Contact lecturer

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Group languages

You can consult this information at the [end](#) of the document.

Prerequisites

A solid knowledge of the subjects in mathematics studied in secondary education (including "batxillerat") is required, as well as a solid basis of the competencies corresponding to the first-semester course "Matemàtiques I".

Objectives

The course has three fundamental parts: the differential calculus, integral calculus and vector analysis.

The objectives of the course are:

(i) Understand the basic concepts in each of these sections. These concepts include both the definitions of the mathematical objects that are introduced and the relationships between them. In other words, it is necessary to understand and know the key points that will be covered in the theory lectures.

(ii) To be able to apply the concepts studied coherently to the approach and resolution of problems.

(iii) Acquire skills in mathematical writing and in calculus.

Learning outcomes

- CM04 (Propose the optimal mathematical tools for solving problems in the field of Chemistry.) Propose the optimal mathematical tools for solving problems in the field of Chemistry.
- CM05 (Solve real, basic mathematical problems applied to chemistry and, to a lesser extent, to other scientific fields.) Solve real, basic mathematical problems applied to chemistry and, to a lesser extent, to other scientific fields.
- KM04 (Identify the presence of underlying mathematics in science, with special emphasis on chemistry, taking into account analytical thinking, abstraction, and logical and rigorous reasoning.) Identify the presence of underlying mathematics in science, with special emphasis on chemistry, taking into account analytical thinking, abstraction, and logical and rigorous reasoning.
- KM05 (Identify elementary mathematical models and tools for calculus, linear algebra, and differential equations.) Identify elementary mathematical models and tools for calculus, linear algebra, and differential equations.
- KM06 (Describe the concepts of numerical methods: precision, discretisation, numerical error, conditioning and normalisation for use in solving physical problems.) Describe the concepts of numerical methods: precision, discretisation, numerical error, conditioning and normalisation for use in solving physical problems.
- SM05 (Analyse the mathematical nature of certain chemical phenomena by abstracting essential variables and formulating mathematical models to describe them.) Analyse the mathematical nature of certain chemical phenomena by abstracting essential variables and formulating mathematical models to describe them.
- SM06 (Use mathematical calculations to solve simple problems in the field of Chemistry and, to a lesser extent, in other scientific fields.) Use mathematical calculations to solve simple problems in the field of Chemistry and, to a lesser extent, in other scientific fields.
- SM07 (In the field of Chemistry, use graphic and numerical methods in the exploration, description and interpretation of mathematical data.) In the field of Chemistry, use graphic and numerical methods in the exploration, description and interpretation of mathematical data.

Contents

(0) Reminder of fundamental concepts (composition of functions, notation, etc).

(1) Functions of several variables

- Geometry of the plane and space.
- Parametric curves. Tangent vector to a curve at a point. Length of a curve.
- Graph of a function, curves, and level surfaces.
- Directional derivatives, gradient.
- Differentiability. Chain rule. Higher-order derivatives. Absolute and relative extrema.

- Critical points, saddle points. Hess's criterion for relative extrema. Lagrange multipliers for absolute extrema.

(2) Multiple integrals.

- Iterated integrals. Fubini's theorem. Cavalieri's principle.
- Change of variable theorem. Polar, cylindrical, and spherical coordinates. Calculation of masses and centers of mass.

(3) Integrals over curves and surfaces.

- Line integrals.
- Parametric surfaces. Tangent planes, normal vectors, and area of a surface.
- Surface integrals and flux of a vector field.
- Green's, Gauss's, and Stokes's theorems.

Learning activities and methodology

Title	Hours	ECTS	Learning outcomes
Problems	22	0.88	
Theory	25	1	
Study	39	1.56	
Solving problems	39	1.56	
Tutorials	12	0.48	
Seminars	2	0.08	

Lectures where definitions, initial results and examples are presented. It is necessary to study the theoretical results covered in these sessions, as they will form the core content of the assessment tests.

Problem-solving sessions where these examples are explored in depth, and where students are expected to attempt to solve the problems independently before attending the session.

To achieve a positive result in this module, it is highly recommended to follow the following steps when preparing for your studies:

- (i) Read the theory notes posted on the Virtual Campus beforehand. Identify any concepts that you may find more difficult.
- (ii) Attend the corresponding theory sessions. Students are expected to participate actively, asking any questions they may have at all times. All questions are welcome (and encouraged) during the theory sessions.
- (iii) Reading and attempting to solve the corresponding problems. It is strongly recommended to first make an active, individual effort to solve the problems. In a second iteration, working in groups to solve the problems is a good idea. Finally, once you have attempted them individually and as a group, you may resort to (though it is by no means essential) AI tools for assistance. It is important not to alter this order of operations and not to start by using this tool directly. In fact, for this module, it is recommended to avoid using generative Artificial Intelligence tools, as current models tend to agree with and confirm the user's hypotheses, which can create a false sense of mastery over the subject matter.
- (iv) Attendance at the problem-solving sessions corresponding to this block. Active participation from students is expected, asking any questions they may have at all times. All questions are welcome (and encouraged) during the problem-solving sessions.

Annotation: within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Assessment

Continuous assessment activities

Title	Weight	Hours	ECTS	Learning outcomes
Seminar	10%	2	0.08	CM04, CM05, KM04, KM05, KM06, SM05, SM06, SM07
Midterm Exam	40%	3	0.12	CM04, CM05, KM04, KM05, KM06, SM05, SM06, SM07
Final Exam	50%	3	0.12	CM04, CM05, KM04, KM05, KM06, SM05, SM06, SM07
Recovery Exam	90%	3	0.12	CM04, CM05, KM04, KM05, KM06, SM05, SM06, SM07

During the course, 3 assessment components will be evaluated:

1. During problem-solving classes and/or seminars, the content of certain sessions will be assessed. These sessions will be announced sufficiently in advance. This results in a grade S.
2. A midterm exam will be held approximately halfway through the semester, resulting in a grade P1.

A second midterm exam covering the course content not assessed in the first midterm will be held at the end of the semester, resulting in a grade P2. If $\min(P1, P2) < 3.5$, the student must take the resit examination. Otherwise, the final grade is calculated using the formula $N1 = 0.1 \cdot S + 0.4 \cdot P1 + 0.5 \cdot P2$. If $N1 < 5$, the student must take the resit examination. If $N1 \geq 5$, the student passes the course with a final grade of N1.

For the resit examination, four possible cases are distinguished:

(a) If $\max(P1, P2) < 3.5$, the student must take a comprehensive resit examination, resulting in a grade R. In this case, the final course grade will be $N = 0.1 \cdot S + 0.9 \cdot R$.

(b) If condition (a) is not satisfied and $P1 < 3.5$, the student has two options and must choose one on the day of the examination.

Option (b1): Take a resit examination for the first midterm, resulting in a grade R1, and obtain a final course grade of $N = 0.1 \cdot S + 0.4 \cdot R1 + 0.5 \cdot P2$.

Option (b2): Take a full resit examination, resulting in a grade R, and obtain a final course grade of $N = 0.1 \cdot S + 0.9 \cdot R$.

(c) If neither condition (a) nor (b) is satisfied and $P2 < 3.5$, the student has two options and must choose one on the day of the examination.

Option (c1): take a resit examination for the second midterm, resulting in a grade R2, and obtain a final course grade $N = 0.1 \cdot S + 0.4 \cdot P1 + 0.5 \cdot R2$.

Option (c2): take a full resit examination, resulting in a grade R, and obtain a final course grade $N = 0.1 \cdot S + 0.9 \cdot R$.

(d) If neither condition (a), (b), nor (c) is satisfied (that is, $P1 \geq 3.5$ and $P2 \geq 3.5$, but $N1 < 5$), the student has three options and must choose one on the day of the examination.

Option (d1): take a resit examination for the first midterm, resulting in a grade R1, and obtain a final course grade $N = 0.1 \cdot S + 0.4 \cdot R1 + 0.5 \cdot P2$.

Option (d2): take a resit examination for the second midterm, resulting in a grade R2, and obtain a final course grade $N = 0.1 \cdot S + 0.4 \cdot P1 + 0.5 \cdot R2$.

Option (d3): take a full resit examination, resulting in a grade R, and obtain a final course grade $N = 0.1 \cdot S + 0.9 \cdot R$.

In the case of partial resits, the resit grade will only be considered if a minimum score of 3.5 is obtained in the resit component. Thus, in cases (b1) and (d1), $R1 > 3.5$ is required, and in cases (c1) and (d2), $R2 > 3.5$ is required. If this minimum score is not achieved, the course will be considered failed with a final grade of $\min(N, 4.5)$. "Cum Laude" grading is not accessible through the resit examination.

Students who have opted for the single-assessment modality must complete an oral theory examination and a final written examination covering the entire course syllabus. These will take place on the same day that continuous-assessment students take the second midterm examination. The student's final grade will be the average of these two assessments.

Students will be considered Not Assessed if they attend only one or none of the assessment activities.

Any irregularity committed during any of the assessment activities described above (academic fraud, plagiarism, or improper use of AI) will result in a grade of 0 for that assessment activity. If multiple irregularities occur across different assessment activities, the final grade for the course will be 0. In addition, disciplinary proceedings may be initiated against any student who commits such irregularities.

Bibliography

Notes adapted to the course will be available on the "Campus Virtual".

Other books to delve deeper into the subject are the following:

1. J. E. Marsden y A.J. Tromba. Cálculo vectorial, cuarta edición. Addison-Wesley Longman, 1998.
2. S. L. Salas y E. Hille. Calculus, Vol. 1 y 2, tercera edición. Reverté, Barcelona, 1995 y 1994.
3. B. Demidovich. Problemas y ejercicios de Análisis Matemático. Ed. Paraninfo.

Software

Does not apply.

Course groups and languages

The information provided is provisional until November 30. After this date, you will be able to consult the language of each group through this [link](#). To access the information, you will need to enter the course CODE

Type of teaching	Group	Language	Semester	Shift
(TE) Theory	1	Catalan/Spanish	second semester	morning-mixed

(PAUL) Classroom practices	1	Catalan/Spanish	second semester	morning-mixed
(SEM) Seminars	1	Catalan/Spanish	second semester	morning-mixed
(TE) Theory	2	Catalan/Spanish	second semester	afternoon
(PAUL) Classroom practices	2	Catalan/Spanish	second semester	morning-mixed
(SEM) Seminars	2	Catalan/Spanish	second semester	morning-mixed
(PAUL) Classroom practices	3	Catalan/Spanish	second semester	afternoon
(SEM) Seminars	3	Catalan/Spanish	second semester	afternoon
(PAUL) Classroom practices	4	Catalan/Spanish	second semester	afternoon
(SEM) Seminars	4	Catalan/Spanish	second semester	afternoon