COURSE SYLLABUS

1. Information regarding the programme

1.1 Higher education institution	Babeș-Bolyai University of Cluj-Napoca
1.2 Faculty	Chemistry and Chemical Engineering
1.3 Department	Chemistry and Chemical Engineering, Hungarian Line of Study
1.4 Field of study	Chemical Engineering
1.5 Study cycle	Master
1.6 Study programme / Qualification	Chemistry and engineering of nano- and biomaterials

2. Information regarding the discipline

2.1 Name of the discipline			**Numerical Methods in Engineering (in English)** CME7325				
2.2 Course coordinator			Lecturer dr. Nagy Levente Csaba				
2.3 Seminar coordinator			Lecturer dr. Nagy Levente Csaba				
2.4. Year of study	I	2.5 Semester	2	2.6. Type of evaluation	C	2.7 Type of discipline	DS

3. Total estimated time (hours/semester of didactic activities)

3.1 Hours per week	4	Of which: 3.2 course	2	3.3 seminar/laboratory	2
3.4 Total hours in the curriculum	56	Of which: 3.5 course	28	3.6 seminar/laboratory	28
Time allotment:					hours
Learning using manual, course support, bibliography, course notes					25
Additional documentation (in libraries, on electronic platforms, field documentation)					18
Preparation for seminars/labs, homework, papers, portfolios, and essays					20
Tutorship					3
Evaluations					3
Other activities:					-

3.7 Total individual study hours	69
3.8 Total hours per semester	125
3.9 Number of ECTS credits	5

4. Prerequisites (if necessary)

4.1. curriculum	• Basic Chemical Engineering
4.2. competencies	• Basic computer skills (Octave or Matlab)

5. Conditions (if necessary)

5.1. for the course	• Room with multimedia projector, projection screen, internet access. • Mobile phones on silent mode.
5.2. for the seminar /lab activities	• Multimedia projector, projection screen, internet access. • Laboratory equipped with computers and specific software. Students work individually at a workstation. • Students will arrive on time and attend the lab with their cell phones on silent mode. All lab hours and seminar are compulsory.

6. Specific competencies acquired

Professional competencies	• Understanding of the numerical methods used for solving various problems in the field of chemical engineering. • Use of numerical calculation tools (Mathematica, MATLAB) • Data analysis and correct interpretation of numerical results. • Creative use of analysis and synthesis in algorithm development. • Identification and application of concepts, methods, and theories to solve engineering problems under skilled assistance conditions. • Use of language, mathematical modeling concepts and programming techniques using general purpose and chemical engineering specific programming languages.
Transversal competencies	• Ability of systemic thinking, holistic thinking, critical thinking, argumentative, problem-solving orientation, high level of computer skills. • Application of efficient work rules and responsible attitudes towards the scientific domain, for the creative exploitation of one's own potential according to the principles and rules of professional ethics • Efficient conduct of activities organized in an interdisciplinary group and development of empathic capacity of interpersonal communication, networking and collaboration with diverse groups. • Use of efficient methods and techniques for learning, information, research and development of abilities for knowledge exploitation, for adapting to the needs of a dynamic society and for communication in a widely used foreign language.

7. Objectives of the discipline (outcome of the acquired competencies)

7.1 General objective of the discipline	• Familiarity with numerical methods with applications in the field of chemical engineering. • Deepening the knowledge acquired in the course and acquiring practical knowledge related to the field. • The ability to use computer tools in solving mathematical models associated with chemical engineering problems, especially specialized technical-scientific calculation programs.
7.2 Specific objective of the discipline	• The ability to abstract and create algorithms for solving problems in numerical form. • The ability to formulate mathematical models specific to chemical engineering, to formulate numerical models appropriate to each situation, to select the most suitable solution methods and to use the computer both to solve the models and to interpret the numerical data obtained.

8. Content

8.1 Course	Teaching methods	Remarks
8.1.1. Presentation of the discipline. Representation of numbers. Errors in numerical calculations. Numerical error analysis. Truncation and rounding errors. Accuracy and precision.	Presentation. Explanation. Practical examples. Case-study discussions.	2 hours

8.1.2. Numerical solution of algebraic and transcendental equations I. Separation of roots. Bisection and secant method.	Presentation. Explanation. Practical examples. Case-study discussions.	2 hours
8.1.3. Numerical solution of algebraic and transcendental equations II. Newton's method. The method of successive approximations.	Presentation. Explanation. Practical examples. Case-study discussions.	2 hours
8.1.4. Systems of linear equations and matrix methods. Direct methods. The Thomas algorithm. Iterative methods (Jacobi, Gauss-Seidl, successive relaxations).	Lecture Computer simulations Power point presentations Interactive exercises	2 hours
8.1.5. Numerical calculation of vectors and eigenvalues (power method). Matrix factorization.	Lecture Computer simulations Power point presentations Interactive exercises	2 hours
8.1.6. Nonlinear equations and systems of equations. Fixed point method. Newton's method.	Lecture Computer simulations Power point presentations Interactive exercises	2 hours
8.1.7. Interpolation and numerical approximation of functions I. Polynomial interpolation (Lagrange, Newton, Hermite, Chebyshev). Approximation of functions by least squares.	Lecture Computer simulations Power point presentations Interactive exercises	2 hours
8.1.8. Interpolation and numerical approximation of functions II. Polynomial interpolation (Lagrange, Newton, Hermite, Chebyshev). Analysis of polynomial interpolation. Interpolation with cubic spline functions.	Lecture Computer simulations Power point presentations Interactive exercises	2 hours
8.1.9. Numerical differentiation and integration of functions I. Newton-Cotes formulas (rectangle rule, trapezoid rule).	Lecture Computer simulations Power point presentations Interactive exercises	2 hours
8.1.10. Differentiation and numerical integration of functions II. The Simpsons Rules. Gauss quadrature.	Lecture Computer simulations Power point presentations Interactive exercises	2 hours
8.1.11. Numerical integration of ordinary differential equations I. Methods for one-step initial value problems (Taylor series development method, Euler method, Runge-Kutta methods).	Lecture Computer simulations Power point presentations Interactive exercises	2 hours
8.1.12. Numerical integration of ordinary differential equations II. Methods for multistep initial value problems (explicit and implicit). Numerical solution of systems of ordinary differential equations. Boundary value problems.	Lecture Computer simulations Power point presentations Interactive exercises	2 hours
8.1.13. Numerical integration of equations with partial derivatives. Numerical methods for problems with parabolic equations. Practical application.	Lecture Computer simulations Power point presentations Interactive exercises	2 hours

8.1.14. Numerical integration of equations with partial derivatives. Numerical methods for problems with elliptic and hyperbolic equations. Practical application.	Lecture Computer simulations Power point presentations Interactive exercises	2 hours

Bibliography

1. A. Constantinides, N. Mostoufi, *Numerical methods for chemical engineers with MATLAB applications*. Prentice Hall, **1999**.
2. C.L. Nagy, *Suport de curs în format electronic*.
3. I. Faragó, R. Horváth, *Numerikus módszerek*. ELTE TTK, BME TTK, **2013**.
4. N. Ghasem, *Numerical methods in chemical engineering using python® and simulink®*. CRC Press, **2023**.
5. K.D. Dorfman, P. Daoutidis, *Numerical methods with chemical engineering applications*. Cambridge University Press, **2017**.

8.2 Seminar / laboratory	Teaching methods	Remarks
8.2.1. Numerical solution of algebraic and transcendental equations.	Explanation. Interactive discussions	2 hours
8.2.2. Numerical solution of systems of linear equations by direct and iterative methods.	Explanation. Interactive discussions	2 hours
8.2.3. Numerical calculation of vectors and eigenvalues.	Explanation. Interactive discussions	2 hours
8.2.4. Application of Lagrange, Newton, Hermite, Chebyshev methods in polynomial interpolation.	Explanation. Interactive discussions	2 hours
8.2.5. Numerical differentiation and numerical integration using Simpson's rule.	Explanation. Interactive discussions	2 hours
8.2.6. Numerical integration by Newton-Cotes and Gauss type formulas.	Explanation. Interactive discussions	2 hours
8.2.7. Numerical integration of ordinary differential equations with the explicit and implicit Euler method.	Explanation. Interactive discussions	2 hours
8.2.8. Numerical integration of ordinary differential equations with Runge-Kutta methods.	Explanation. Interactive discussions	2 hours
8.2.9. Numerical integration of ordinary differential equations with the Taylor method.	Explanation. Interactive discussions	2 hours
8.2.10. Numerical solution of systems of ordinary differential equations with boundary values by shooting and finite difference methods.	Explanation. Interactive discussions	2 hours
8.2.11. Numerical integration of parabolic partial differential equation problems.	Explanation. Interactive discussions	2 hours
8.2.12. Numerical integration of elliptic partial differential equation problems.	Explanation. Interactive discussions	2 hours
8.2.13. Use of numerical calculation tools I. Introduction to Mathematica.	Explanation. Interactive discussions	2 hours
8.2.14. Use of numerical calculation tools II. Introduction to Python.	Explanation. Interactive discussions	2 hours

Bibliography

1. A. Constantinides, N. Mostoufi, *Numerical methods for chemical engineers with MATLAB applications*. Prentice Hall, **1999**.
2. C.L. Nagy, *Suport de curs în format electronic*.
3. I. Faragó, R. Horváth, *Numerikus módszerek*. ELTE TTK, BME TTK, **2013**.
4. N. Ghasem, *Numerical methods in chemical engineering using python® and simulink®*. CRC Press, **2023**.
5. K.D. Dorfman, P. Daoutidis, *Numerical methods with chemical engineering applications*. Cambridge University Press, **2017**.
6. H.C. Foley, *Introduction to chemical engineering analysis using Mathematica*. Academic Press, **2002**.

9. Corroborating the content of the discipline with the expectations of the epistemic community, professional associations, and representative employers within the field of the program

The acquisition of the theoretical-methodological concepts and the approach of the practical aspects included in the Process Intensification discipline the will students acquire a consistent knowledge bag in accordance with the competencies of the Diploma Supplement and the qualifications of the ANC.

10. Evaluation

Type of activity	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Share in the grade (%)
10.4 Course	Acquiring and understanding of the course content information	Exam	75
10.5 Seminar/lab activities	Learning and understanding of issues addressed in the seminar / laboratory	Quality of solved homework	25
10.6 Minimum performance standards			
• Grade 5 (five) at the exam. • Knowledge of introductory notions; experimental data processing.			

Date
April 5, 2024

Signature of course coordinator
Lect. dr. NAGY Levente Csaba

Signature of seminar coordinator
Lect. dr. NAGY Levente Csaba

Date of approval
April 15, 2024

Signature of the Director of the Department
Prof. Habil. dr. eng. Paizs Csaba