

ChE-312

Numerical methods

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Cursus	Sem.	Type
Chemical Engineering	BA6	Obl.
Chemistry	BA6	Obl.
HES - CGC	E	Opt.

Language of teaching	English
Credits	3
Session	Summer
Semester	Spring
Exam	Written
Workload	90h
Weeks	14
Hours	3 weekly
Courses	2 weekly
Exercises	1 weekly
Number of positions	

Summary

This course introduces students to modern computational and mathematical techniques for solving problems in chemistry and chemical engineering. The use of introduced numerical methods will be demonstrated using the MATLAB programming language.

Content

- Numerical differentiation (Euler forward, backward, Richardson extrapolation, error analysis)
- Numerical integration (Trapezoid rule, Simpson rule, composite rules, Romberg integration)
- Methods for solving nonlinear equations (bisection, Regula-Falsi, Newton-Raphson, error analysis)
- Methods for solving ordinary differential equations (notion of stability of solutions, stiffness, Euler methods, Runge-Kutta methods, Adams-Bashfort-Moulton, adaptive methods)
- Boundary value problems (finite difference method, FTCS scheme, Crank-Nicolson method, Finite difference methods in 2 and 3 spatial dimensions, Transient Boundary value problems)
- Basic notions of data analysis/processing

Keywords

Numerical differentiation and integration, nonlinear equations, ordinary differential equations, partial differential equations

Assessment methods

The final grade will be the combination of exercises (30%) and written exams (70%)