CH-250

# Numerical methods in chemistry

Miskovic Ljubisa, Vanicek Jiri

| Cursus | Sem. | Type |
|---|---|---|
| Chemistry and chemical engineering | BA3 | Obl. |
| HES - CGC | H | Obl. |

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|---|---|
| Language of teaching | English |
| Credits | 4 |
| Session | Winter |
| Semester | Fall |
| Exam | During the semester |
| Workload | 120h |
| Weeks | 14 |
| **Hours** | **4 weekly** |
| Courses | 2 weekly |
| Exercises | 2 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

*Part I*
Basic features of Matlab: scripts, functions, variables, expressions, visualization
Methods for solving linear equations
Methods for solving non-linear equations
Methods for solving ordinary differential equations (ODE) and differential-algebraic equations (DAE)
Basic tools in data analysis
*Part II*
Laplace transform, convolution, and solution of ordinary differential equations
Fourier series, separation of variables, and solution of partial differential equations
Fourier transform
Applications of integral transforms in chemical engineering and physical chemistry

## Learning Outcomes

By the end of the course, the student must be able to:

- Solve numerically various problems in chemistry and chemical engineering
- Use fluently the MATLAB programming language
- Work out / Determine analytically Laplace and Fourier transforms, Fourier series, and convolutions of functions
- Apply integral transforms to solve analytically or numerically differential equations and other problems in chemistry and chemical engineering

## Assessment methods

Part I (Miskovic): homeworks 50% + midterm exam 50%
Part II (Vanicek): homeworks 30% + midterm exam 70%
The points from the two parts are combined to form the final grade.

## Supervision

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| Office hours | Yes |
| Assistants | Yes |

## Resources

## Bibliography

1. S. Attaway, MATLAB – A practical introduction to programming and problem solving
2. P. Dyke, An introduction to Laplace transforms and Fourier series, Springer, 2014

## Ressources en bibliothèque

- An introduction to Laplace transforms and Fourier series / Dyke
- MATLAB : a practical introduction to programming and problem solving / Attaway