

## Mathematical Methods in Chemical Technology (E002620)

Course size (nominal values; actual values may depend on programme)

Credits 6.0 Study time 180 h Contact hrs 60.0 h

Course offerings and teaching methods in academic year 2018-2019

A (semester 1)	Dutch	seminar: practical PC room classes	15.0 h
		seminar: coached exercises	15.0 h
		lecture	30.0 h

Lecturers in academic year 2018-2019

Constales, Denis TW16 lecturer-in-charge

Offered in the following programmes in 2018-2019

	crdts	offering
<a href="#">Master of Science in Chemical Engineering</a>	6	A
<a href="#">Master of Science in Chemical Engineering</a>	6	A

Teaching languages

Dutch

Keywords

Position of the course

We deal with several topics from mathematical analysis, which are not covered by Analysis I-III in the bachelor, but have applications in chemical engineering problems, such as chromatography and chemical reactor theory. These practical applications will appear in illustrative examples throughout the theory as well as in the exercise sessions.

Contents

- Calculus of variations: First problem of the calculus of variation, Constrained extrema problems, Extension to multiple variables
- Analytical methods for boundary-value problems: Generalized Fourier transform methods, Green's function methods
- First order partial differential equations: Method of characteristics, Shocks and weak solutions
- Uniqueness of linear and nonlinear systems: Maximum principles, Energy methods
- Perturbation methods: Regular perturbation methods, Singular perturbation problems
- Inverse methods: Examples of inverse problems, Approximate recovery of missing data, Minimization of the "cost functional"

Initial competences

Analysis I and II

Final competences

- 1 Knowledge of the concepts of extremals, differential equations of Euler-Lagrange; side condition in integral form, algebraic side condition; characteristics of a first order partial differential equation; weak solution of a first order partial differential equation; extremal values of solutions; maximum principles; method of Ritz; perturbation parameter in a differential equation, unperturbed problem.
- 2 Insight in the necessary conditions for an extremum; multiplier method of Lagrange; eigenvalue problems, Fourier method for time dependent boundary value problems; integral form of the analytical solution; construction of Green's functions; convergence of iteration methods; development of the solution in terms of the perturbation parameter.

#### Conditions for credit contract

Access to this course unit via a credit contract is determined after successful competences assessment

#### Conditions for exam contract

This course unit cannot be taken via an exam contract

#### Teaching methods

Lecture, seminar: coached exercises, seminar: practical PC room classes

#### Learning materials and price

Syllabus and materials on Minerva.

#### References

- A. Varma and M. Morbidelli, *Mathematical Methods in Chemical Engineering*, Oxford University Press, New York, 1997
- S. Pushpavanam, *Mathematical Methods in Chemical Engineering*, Prentice Hall of India, New Delhi, 2005
- N.W. Loney, *Applied mathematical methods for chemical engineers*, Boca Raton , CRC Press, 2006.

#### Course content-related study coaching

Individual consulting after the lectures or via email or appointments.

#### Evaluation methods

end-of-term evaluation

#### Examination methods in case of periodic evaluation during the first examination period

Written examination with open questions

#### Examination methods in case of periodic evaluation during the second examination period

Written examination with open questions

#### Examination methods in case of permanent evaluation

#### Possibilities of retake in case of permanent evaluation

not applicable

#### Calculation of the examination mark