

Chemistry of Industrial Processes (E071181)

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 2016-2017

A (semester 2)	integration seminar	47.5 h
	seminar	5.0 h
	guided self-study	22.5 h
B (semester 2)	lecture	22.5 h
	seminar	5.0 h
	integration seminar	47.5 h

Lecturers in academic year 2016-2017

Reyniers, Marie-Françoise	TW11	lecturer-in-charge
Van Speybroeck, Veronique	TW17	co-lecturer

Offered in the following programmes in 2016-2017

	crdts	offering
Bridging Programme Master of Science in Chemical Engineering	6	B
Bridging Programme Master of Science in Chemical Engineering	6	A
Master of Science in Electromechanical Engineering (main subject Control Engineering and Automation)	6	B
Master of Science in Electromechanical Engineering (main subject Electrical Power Engineering)	6	B
Master of Science in Electromechanical Engineering (main subject Maritime Engineering)	6	B
Master of Science in Electromechanical Engineering (main subject Mechanical Construction)	6	B
Master of Science in Electromechanical Engineering (main subject Mechanical Energy Engineering)	6	B
Master of Science in Chemical Engineering	6	B
Master of Science in Sustainable Materials Engineering	6	B
Master of Science in Chemical Engineering	6	A

Teaching languages

Dutch, English

Keywords

industrial chemical processes, reaction mechanisms, sustainable chemistry

Position of the course

Analysis of the reaction mechanisms involved in large scale chemical processes. Getting acquainted with the application of molecular level insights for the optimization and development of sustainable chemical processes in (petro)chemistry, fine chemistry and polymer chemistry.

Contents

- Equilibrium constants and reaction rates
 - Molecular partition functions and derived thermodynamic properties
 - Equilibrium constants from ab initio data
 - Reaction rates from ab initio data
 - Accuracy of thermodynamic and kinetic properties

- Acid catalyzed processes:
 - Conversion of renewable resources
 - sensitivity analysis
 - reaction path analysis
- Metal catalysed processes:
 - First principles based catalyst and reactor design
 - Ammonia production
 - CO oxidation
 - mean field approximation versus kinetic Monte Carlo

Initial competences

Organic chemistry, Physical chemistry, Polymers, Surface phenomena and catalysis, Chemistry and sustainable technology

Final competences

- 1 NOTIONS: reaction families, linear free energy relations, vulcano curve, optimal catalyst curves, microkinetic modelling, kinetic parameters, catalyst descriptors
- 2 SKILLS: application of molecular level insights for process optimization and development

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

Guided self-study, lecture, project, seminar

Extra information on the teaching methods

The lectures consist of theoretical lessons (~40) in which case studies are used to present and illustrate concepts. In the project sessions (~24) projects are worked out. In essence the solution to given problems is obtained and discussed during the project sessions, contrary to the coached exercises (~4) in which during the contact hours an introduction is given and it is expected that the student fulfills the tasks independently. For the seminar projects a brief report is expected (individually or per group of 4-5 students)

Learning materials and price

English syllabus; electronically available on Minerva

References

ULLMANN'S Encyclopedia of Industrial Chemistry: <http://www.wiley-vch.de/vch/software/ullmann/>

Course content-related study coaching

Lecturer and assistant are available after appointment for extra explanation about the course and for feedback on the evaluations

Evaluation methods

end-of-term evaluation and continuous assessment

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

Oral examination

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

Oral examination

Examination methods in case of permanent evaluation

Oral examination

Possibilities of retake in case of permanent evaluation

examination during the second examination period is not possible

Extra information on the examination methods

- Periodic evaluation: oral exam (open-book), written preparation
- Permanent evaluation: quotation of presentation; Second examination: not possible
- Frequency: 3 seminar project presentation

Calculation of the examination mark

- Permanent and periodic evaluation