GHENT UNIVERSITY

Course Specifications

From the academic year 2015-2016 up to and including the

Chemical Reactors: Fundamentals and Applications (E072110)

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	guided self-study	30.0 h
		group work	3.75 h
		integration seminar	2.5 h
		seminar: coached exercises	6.25 h
		seminar: practical PC room classes	6.25 h
		project	3.75 h
		practicum	7.5 h
		excursion	7.5 h
B (semester 1)	English	seminar: coached exercises	6.25 h
		project	3.75 h
		integration seminar	2.5 h
		practicum	7.5 h
		group work	3.75 h
		seminar: practical PC room classes	6.25 h
		excursion	7.5 h
		lecture	30.0 h

Lecturers in academic year 2018-2019

Marin, Guy	TW11	lecturer-in-charge
Van Steenberge, Paul	TW11	co-lecturer

Offered in the following programmes in 2018-2019	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 Chemical Engineering	6	A

Teaching languages

Dutch, English

Keywords

Stoichiometry, kinetics, thermodynamics, transport limitations, heterogeneous catalysis, tubular reactors, packed bed reactors, fluidized bed reactors, gas liquid reactors, continuous flow reactors, batch reactors, residence time distribution, reactor stability,

adiabatic reactors, non-isothermal reactors

Position of the course

Relying on course units such as ‘Physical Chemistry (E029010)’, ‘Heat Engineering and Mass Transport (E045910)’ and ‘Surface Phenomena and Catalysis (E071161)’, the first part of this course unit introduces the concepts applied to the mathematical design of major chemical reactor types used in the chemical process industry. A second part of this course unit encompasses the application of these concepts to the most important of these reactor types. The competences acquired during this course unit correspond to the initial competences of the course unit "Safety and Environment" (E072301), in which safety and environmental aspects of chemical reactors and processes are taught.

Contents

- Lectures:
  - Isothermal reactors with ideal flow pattern: batch reactor with ideal mixing, steady state plug flow reactor, steady state continuous stirred tank reactor, cascade of CSTRs
  - Isothermal continuous reactors with non-ideal flow pattern: relation between flow pattern and residence time distribution, effect of the residence time distribution on the conversion, micromixing, macromixing, models for non-ideal flow
  - Stoichiometry: elementary reactions, complex reactions
  - Thermodynamics of chemical reactions: reaction enthalpy, chemical equilibrium
  - Kinetics: definitions, kinetics of elementary reactions, kinetics of global reactions
  - Non-isothermal reactors with ideal flow pattern: enthalpy production, maximum isobaric adiabatic temperature variation, batch reactor, steady state plug flow reactor, steady state continuous stirred tank reactor
  - Transport phenomena: introduction, reaction and transport in series, simultaneous reaction and transport, combination of external and internal transport limitations, gas liquid reactions
  - Experimental study of heterogeneously catalyzed reactions: introduction, reactor types, differential versus integral operation, criteria for the negligibility of transport phenomena on pellet scale, construction of rate equations
  - Tubular reactors: introduction, model equations, physical parameters
  - Packed bed reactors: model classification, ideal pseudohomogeneous one-dimensional model, pseudohomogeneous one-dimensional model with effective axial diffusion and conduction, pseudohomogeneous two-dimensional model for plug flow with effective radial diffusion and conduction, one-dimensional heterogeneous model
  - Gas liquid reactors: introduction, perfectly mixed gas and liquid phase, gas and liquid phase in plug flow
  - Fluidized bed reactors: introduction, fluidization phenomenon, fluidization regimes, two-phase model for fluidized bed reactors
  - Q&A session
- Seminars
  - Isothermal reactors
  - Stoichoimetry, thermodynamics and kinetics
  - Non-isothermal reactors
  - Transport phenomena
  - Bench scale reactors and packed bed reactors
  - Simulation of flow fields in reactors I
- Integration seminar
  - Assessment of intrinsic kinetics in fixed bed reactors
- Projects and group work
  - Simulation of a tubular reactor
  - Simulation of a gas liquid reactor
  - Simulation of flow fields in reactors II
- Practical
  - Hydroisomerization
  - Thermal cracking
- Study visit: Industrial reactors

Initial competences

Informatics (E015040)
Mathematical Analysis I: Functions of One Variable (E001130)
Geometry and Linear Algebra (E000660)
Physical Chemistry (E029010)
Heat Engineering and Mass Transport (E045910)
Introduction to Numerical Mathematics (E002910)

Basis Mathematics Tools (E001140)
Surface Phenomena and Catalysis (E071161)

Final competences

1 **KNOWLEDGE: CONCEPTS**
Defining: conversion, selectivity, yield, batch reactor, plug flow reactor, continuous stirred
tank reactor (CSTR), residence time distribution, stoichiometric coefficients, degree of advancement, key component, affinity, maximal isobaric adiabatic temperature rise, effectiveness factor, enhancement factor, Thiele modulus, Hatta number, intrinsic kinetics, axial and radial mixing, internal and external gradients, fluidization, bubble formation, effective diffusion, micromixing, macromixing

2 **KNOWLEDGE: INSIGHTS:**
Deriving, calculating, explaining and predicting of kinetics of single and global reactions,
effects of non-isothermicity on the behavior of different reactor types, diffusion vs. reaction, physical meaning of parameters in model equations

3 **KNOWLEDGE: RELATIONS:**
Deriving, calculating, explaining and predicting: the effect of non-ideal flow patterns on
reactor behavior, temperature dependency on the reaction enthalpy and chemical equilibrium, analogy between heat and mass transfer

4 **KNOWLEDGE: MODELS:**
Defining: pseudo-homogeneous models, heterogeneous models and one-dimensional heterogeneous two-phase models

5 **SKILLS: METHODS:**
- Determining the number of global reactions to convert a given feed to desired products
- Acquiring bench scale data leading to rate equations suitable for reactor design
- Assessing the importance of transport and transfer of mass and energy
- Deriving design equations and estimating the related transport parameters
- Deriving the reactor design equations starting from the conservation laws of mass and energy
- Solving the most common and most simple design equations
- Defining a window of operation and designing a reactor accounting for thermodynamic equilibrium
- Assessing and accounting for deviations from ideal flow patterns

6 **SKILLS: HEURISTICS:**
- Estimating orders of magnitude of quantities important for reactor design
- Assessing of criteria for reactor (model) selection and determining the optimal reactor configuration
- Applying rules for scaling up reactors

7 **SKILLS: PROCEDURES:**
Deriving rate equations based on reaction mechanisms suitable for reactor design

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, excursion, group work, lecture, integration seminar, practicum, project, seminar: coached exercises, seminar: practical PC room classes

Extra information on the teaching methods

- The lectures encompass the theory lessons complemented with numerous examples as well as a Q&A session (questions and answers on course material taught up to that time).
- In the seminars theory is illustrated using coached computer exercises using Maple or Fluent.
- The integration seminar is an interactive coached learning situation, with explicit focus on the integration of content from multiple course units/fields (see position of the course) and knowledge sources (e.g.Perry's Chemical Engineers' Handbook, NIST Database, web tools, …).This encompasses discussion, exercises, brief tasks, etc.
- In the projects focus is on knowledge integration of individual course units (e.g. ‘Introduction to Numerical Mathematics (E002910)’ and ‘Informatics (E015040)’) and lectures, with *reports* (interpretations of computer simulations) as end results. *Reports* are written by groups of 4 to 5 students (see evaluation).
- The practicals encompass the use of a high-throughput setup and a pilot scale steam cracker unit (in development).

- The study visit is an excursion to a Ghent harbor company where a number of important reactor types are operated.

Learning materials and price

Syllabus (electronically available on https://minerva.ugent.be).

References

Course content-related study coaching

Appointments can be made with the lecturer and/or the assistant for additional information with respect to the course and 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

Participation, skills test, report

Possibilities of retake in case of permanent evaluation

examination during the second examination period is not possible

Extra information on the examination methods

Periodic: closed book, theory: oral presentation with written preparation, exercise: only written preparation.
Non-periodic: reports, participation (attendance) during practicals and study visit, skills test.

Calculation of the examination mark

Special conditions: non-periodic 4/20, periodic: 11/20 for theory and 5/20 for exercises.