# Course Specifications

From the academic year 2016-2017 up to and including the

## Polymer Reaction Engineering (E064950)

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

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|---|---|---|---|---|---|
| Credits | 6.0 | Study time | 180 h | Contact hrs | 60.0 h |

Course offerings and teaching methods in academic year 2018-2019

| | | | |
|---|---|---|---|
| A (semester 2) | English | lecture | 30.0 h |
| | | seminar: coached exercises | 15.0 h |
| | | project | 15.0 h |
| B (semester 2) | Dutch | guided self-study | 30.0 h |
| | | seminar: coached exercises | 15.0 h |
| | | project | 15.0 h |

Lecturers in academic year 2018-2019

| | | |
|---|---|---|
| D'hooge, Dagmar | TW11 | lecturer-in-charge |

| Offered in the following programmes in 2018-2019 | crdts | offering |
|---|---|---|
| Bridging Programme Master of Science in Chemical Engineering | 6 | A |
| Bridging Programme Master of Science in Chemical Engineering | 6 | B |
| Master of Science in Chemical Engineering | 6 | A |
| Master of Science in Sustainable Materials Engineering | 6 | A |
| Master of Science in Chemical Engineering | 6 | B |

Teaching languages

Dutch, English

Keywords

polymerization reactors, polymerization kinetics, scale-up

Position of the course

The combined application of the basic concepts of kinetics, thermodynamics, transport phenomena, polymerization chemistry and chemical reactors with as aim the design of industrial polymerization reactors, the study of polymerization processes both at laboratory and industrial reactor scale and the design of functional polymer materials. Case studies are considered per polymerization technique/method.

Contents

- Introduction to polymer reaction engineering (Chapter 1)
  - polymerization classes
  - polymerization techniques
  - polymerization reactors
  - important commercial polymers
  - influence of polymerization conditions on polymer properties
- Step-growth polymerization (Chapter 2)
  - properties of step-growth polymerizations
  - mass transfer in step-growth polymerizations
  - reaction kinetics
  - case studies: modeling of industrial step-growth polymerization process: polyesters and polyamides
- Radical polymerization: homogeneous systems (Chapter 3a)
  - free radical (co)polymerization: basic concepts
  - reaction kinetics: influence of molecular diffusion
  - case stuy: design of free radical bulk polymerization of styrene

- Radical polymerization: precipitation polymerization (Chapter 3b)
  - phase equilibrium
  - mass transfer
  - case study:multi-scale modeling of the high impact polystyrene process
- Radical polymerization: controlled radical polymerisation techniques (Chapter 4)
  - reversible deactivation radical polymerization in the presence of transition metal (complexes) such as atom transfer radical polymerization (ATRP): basic models
  - nitroxide mediated polymerization: basic models
  - reversible addition fragmentation chain transfer polymerization: basic models
  - case study: optimization of initiators for continuous activator regeneration ATRP
- Radical polymerization in suspension (Chapter 5)
  - principle
  - surfactants
  - phase equilibrium
  - mass transfer
  - mixing phenomena
  - morphological aspects: modeling of droplet and grain size distributions
  - scale-up of suspension polymerization reactors
  - case study: modeling and design of the industrial poly(vinyl chloride) production process
- Radical polymerization in emulsion (Chapter 6)
  - principle
  - emulsifiers
  - phase equilibrium
  - mass transfer
  - mixing phenomena
  - morphological aspects
  - scale-up of emulsion polymerization reactors
  - case study: modeling and optimization of industrial production of butadiene nitrile rubbers

- Coordination polymerization (Chapter 7)
  - types of olefines
  - catalysts: Ziegler-Natta catalyst, Philips catalyst, and metallocene catalyst
  - reaction kinetics: “single-site” and “multiple-site” copolymerization
  - internal and external transport limitations
  - case study: modeling of industrial reactors for olefin production: defining optimal polymer reactor configuration
- Control of industrial polymerization reactors (Chapter 8)
  - safety: risk evaluation
  - process control: defining and calculating control actions and schemes
  - case studies

## Initial competences

This course builds on certain concepts taught during the courses "Polymers" and "Heat engineering and mass transport".

## Final competences

1. Knowlegde: describing and defining the following concepts: molar mass distribution; coordination polymerization; free radical polymerization; controlled radical polymerization; suspension polymerization; emulsion polymerization; condensation polymerization; polymerization reactor control; monomer removal; polymerization reactor types; scale-up; nucleation; catalysts; drop distributions; phase equilibrium; solution polymerization; bulk polymerization; method of moments; population balances
2. Knowledge: discussing the relation between functional groups present in polymer molecules and polymerization kinetics, the importance of molecular diffusion and mixing phenomena in polymerization processes on laboratory and industrial reactor scale, the physical meaning of the parameters in the model equations, the most important industrial polymerization processes, the effect of the applied polymerization technique and reactor configuration on the polymerization rate and polymer properties
3. Skills: distinguishing and identifying of polymerization reactors with respect to the final application, applying conservation laws for mass and energy for polymerization processes, evaluating the importance of the polymerization kinetics and transport phenomena on various length and time scales, and assessing typical order of magnitudes related to the design of polymerization reactors.
4. Attitude: being able to solve independently and in a group a design problem within the field of polymer reaction engineering.

## 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: coached exercises

Extra information on the teaching methods

The lectures are used to teach the theoretical background complemented with some practical examples/case studies. For the seminars (about 3), the solution is reached in essence during the seminar. In the coached exercises/projects (about 3), on the other hand, an introduction is given and it is expected that the student fulfills the tasks independently/in group. For at least one of these coached exercises/projects a presentation or report is expected.

Learning materials and price

English syllabus; handouts; electronically available via Minerva (https://minerva.ugent.be)

References

1. Introduction to polymers, R.J. Young, P.A. Lovell, 2011, ISBN 978-0-8493-3929-5
2. Polymer Reaction Engineering, J. Asua, Wiley-Blackwell, 2007 ISBN 978-1-4051-4442-1
3. Handbook of Polymer Reaction Engineering (volume 1 and 2), T. Meyer and J. Keurentjes, Wiley- VCH, 2005 ISBN 3-527-31014-2
4. Principles of Polymerization, G. Odian, Wiley, 2004 ISBN 0-471-27400-3.

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, participation, 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 evaluation: oral exam (closed-book), written preparation
Permanent evaluation: quotation of presentation and/or report; Second examination: not possible
Frequency: maximally three times along the semester

Calculation of the examination mark

Permanent and periodic evaluation
Special conditions: 1/3 permanent evaluation; 2/3 periodic evaluation