GHENT UNIVERSITY

Course Specifications

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

Kinetic Modelling and Simulation (E074200)

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)	English	seminar	20.0 h
		lecture	30.0 h
		project	10.0 h
B (semester 1)	Dutch	seminar	20.0 h
		guided self-study	30.0 h
		project	10.0 h

Lecturers in academic year 2018-2019

Thybaut, Joris	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 Chemical Engineering	6	B

Teaching languages

Dutch, English

Keywords

linear and non linear regression analysis, parameter estimation, experimental design, kinetics, simulation methods

Position of the course

Introduction to mathematical modeling and statistical data analysis to develop adequate kinetic models characterized by their physical meaning and statistical significance. Such kinetic models aim at forming the bridge between the phenomena that occur at the reactor scale and at the molecular scale.

Contents

- Reaction equations: pseudo steady state, rate determining step, quasi equilibrium, Langmuir Hinshelwood/Hougen Watson, Eley Rideal, Mars Van krevelen, microkinetics, Single-Event MicroKinetics (SEMK), kinetic descriptors, catalyst descriptors
- Reactor simulation: batch reactor, continuous stirred tank reactor, plug flow reactor, sets of algebraic equations, differential equations, differential algebraic equations, 2nd order differential equations, time dependent component
- Statistics: basic principles: Distributions, Distribution parameters, Some important distributions, More dimensional distributions, Statistical tests and conclusions
- Linear model: linear regression analysis: Unweighed regression, Weighed regression
- non-linear regression analysis: Algorithms for parameter estimation in non-linear models, Preliminary estimates, Properties of the estimated parameter vector, Temperature dependence of the kinetic parameters, Example: a microkinetic model for the hydrogenation of aroamtic components
- Selection of best regression equation: The "All Possible Regressions" procedure, The "Forward Selection" procedure, The "Backward Elimination" procedure, The "Stepwise Regression" procedure, The "Stagewise Regression" procedure, Residual Analysis
- A posteriori techniques for discrimination between rivaling models: Techniques based

on diagnosis parameters, The likelihood ratio as discriminating agent, The physical chemical significance of the parameters, Globale Fitting potential
- Sequential experimental design for model discrimination: Bayesian sequential discrimination procedures, Non-Bayesian procedures
- Sequential experimental design for precise parameter estimation: Effect of k experiments to be performed on the significance of the parameters, Global criteria for experimental design, Simultaneous planning of k experiments, Individual planning of experiments
- Multi variate regression analysis: Maximum likelihood principle: covariance matrices known, Maximum likelihood principle: covariance matrices unknown
- Contribution analysis, Reaction pathway analysis

Initial competences

The present course unit builds on certain learning outcomes of other course units:
“Wiskundige analyse I: functies van één veranderlijke”/“Mathematical Analysis I: functions of one variable”
- Insight of the mathematical, geometric and physical interpretation of the notions of derivative, differential, integral, improper integral, differentiability and integrability.
- Knowledge of the general solution of a linear differential equation, as well as the lack of a general solution of a non-linear differential equation, to be able to solve specific differential equations and to check the existence and uniqueness conditions for the corresponding initial value problems.
- Assessment of the convergence of numerical series and series of functions.
“Oppervlakfenomenen en katalyse”/“Surface phenomena and catalysis”
- Knowledge of the operating principles of catalysis.
- Derivation of rate equations for catalytic cycles.
- Analysis of the interaction between molecules and the surface of solid materials (sorption phenomena and surface reactions).
“Inleiding tot de numerieke wiskunde”/“Introduction to numerical mathematics”
- Understanding and mastering of standard numerical methods for some basic problems (for systems of algebraic equations, initial problems for ODEs, boundary value problems and Eigen value problems in 1D)
“Waarschijnlijkheidsrekening en statistiek”/“Probability and statistics”
- Understanding and mastering multidimensional random variables and their distributions.
- Calculating the probability of events and the expected value of random variables.
- Understanding and applying methods for (parameter) estimation.
- Performing and interpreting linear regression.
“Meetkunde en lineaire algebra”/“Geometry and linear algebra”
- Manipulation of vectors.
- Insight in the notions of vector space, linear dependence and independence, basis and dimension.
- Understanding the mathematical, physical and geometric meaning of eigenvalues and eigenvectors.
“Fysische scheikunde”/“Physical chemistry”
- Understanding of entropy, enthalpy, free energy, chemical equilibrium expression, Langmuir adsorption and chemical reaction dynamics and transition state.
- Insight in relations between chemical equilibrium and thermodynamic macroscopic variables.
- Operational description and determination of thermodynamic equilibrium.
- Consideration of surfaces in the description of thermodynamic equilibrium.

Final competences

1 Critically evaluate typical complex problems in kinetic modelling and subsequently select a suitable, yet manageable technique which is to be implemented in the relevant software
2 Apply interdisciplinary knowledge, e.g., physical chemistry, kinetics, catalysis, reactor engineering, statistics…, when critically evaluating chemical kinetics problems and proposing suitable solutions
3 Use the acquired expertise and apply the interdisciplinary knowledge to solve ill-defined chemical kinetics problems
4 Design a set of experiments which enables the construction of kinetic models
5 Recognize the strengths and weaknesses of the implemented techniques and critically evaluate the solutions obtained
6 Present the techniques, results and conclusion from kinetic modelling activities in a scientific appropriate and concise, yet complete manner, both orally and written

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 classroom lectures are used to teach the theoretical background complemented with some practical examples. These practical examples are further elaborated in the exercises (6). Essentially, the solution of these exercises is reached during the exercise session itself, incontrast to the projects (3) where an introductory session is organized and where the students are expected to reach the solution in an independent manner. A report on these project is expected on an individual basis or per pair of students.

Learning materials and price

Syllabus (Dutch and English) electronically available through Minerva, also distributed by VTK

References

- 'Applied Linear Statistical Models', by Neter, Kutner, Nachtsheim and Wasserman, McGraw-Hill, 1996
- 'Genetic Algorithms in Search, Optimization and Machine Learning', by D.E. Goldberg, Addison-Wesley, 1989
- 'Design of Experiments in Chemical Engineering', by Lazic, Wiley-VCH, 2004

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

Report

Possibilities of retake in case of permanent evaluation

examination during the second examination period is possible in modified form

Extra information on the examination methods

- During examination period: oral closed-book exam, written preparation
- During semester: graded project reports. Second chance: Possible in adapted form
- Frequency: 3 evaluations throughout the semester

Calculation of the examination mark

Evaluation throughout semester as well as during examination period. Special conditions: 1/3 non period bound evaluation 2/3 period bound evaluation. A minimum of 8/20 is required on both non period and period bound evaluation to pass the entire course.