ChE-403

Chemical engineering of heterogenous reaction

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Cursus	Sem.	Type
Energy minor	H	Opt.
Ing.-chim.	MA1, MA3	Obl.

Language of teaching	English
Credits	3
Session	Winter
Semester	Fall
Exam	Written
Workload	90h
Weeks	14
Hours	**3 weekly**
Courses	2 weekly
Exercises	1 weekly
Number of positions	

Summary

The theoretical background and practical aspects of heterogeneous reactions including the basic knowledge of heterogeneous catalysis are introduced. The fundamentals are given to allow for the use of chemical reactors to study reaction kinetics and test various mechanistic assumptions.

Content

1. Introduction and review

- Course goals
- Review of kinetics, transition state theory and the steady state approximation in catalysis
- Basic types of chemical reactors (Batch, CSTR, Plug flow)

2. Non-ideal flow in reactors

- Residence time distribution (RTD)
- Dispersion models for nonideal reactors (axial and radial dispersion)
- Influence of RTD on reactor performance

3. Heterogeneous catalysis

- Definitions
- Kinetics of elementary steps: adsorption, desorption and surface reaction
- Kinetics of overall reactions
- Evaluations of kinetic parameters

4. Effects of transport limitations on rates of solid-catalyzed chemical reactions

- External transport effects
- Internal transport effects
- Combined internal and external transport effects

5. Microkinetic analysis of catalytic reactions

- Basic concepts
- Case studies including ammonia synthesis and ethylene hydrogenation

Keywords

Reactor design, non-ideal reactors, heterogeneous catalysis, residence time distribution, transport limited reactions and microkinetic analysis.

Learning Prerequisites

Recommended courses

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Learning Outcomes

By the end of the course, the student must be able to:

- Assess / Evaluate reactor performance using design equations
- Represent the variation in product concentrations with reactor residence time
- Compute reaction kinetics, conversions (and yields) for a real tubular reactor from the dispersion model
- Develop the expression of the reaction rate and deduce apparent reaction orders from the experimental data for heterogeneous catalytic reaction
- Hypothesize the adsorption type of a reactant involved in a catalytic reaction
- Propose a reaction mechanism and derive rate equation
- Design reactor and optimal catalyst form, size and morphology for particular industrial application

Transversal skills

- Assess one's own level of skill acquisition, and plan their on-going learning goals.
- Use both general and domain specific IT resources and tools
- Manage priorities.
- Use a work methodology appropriate to the task.

Assessment methods

Two written controls during the semester; each control is based on the assessment via 100 points, totally 200 points; the final grade is calculated as: (total pointsx5 /200 +1); **the threshold is 111**.
For example: (111x5/200+1# 4.0)
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Deux contrôles écrites pendant le semestre; chaque contrôle est basé sur l'évaluation par 100 points, totalement 200 points; la note finale est calculée comme la suite: (points x 5 /200+1);
par exemple : (111x5/200+1# 4.0)

Resources

Bibliography

The book for the class will be: Fundamentals of Chemical Reaction Engineering, Frist Ed., by Davis and Davis, McGraw-Hill, New York, 2003.
The book is available for free at the following website: http://authors.library.caltech.edu/25070/

Ressources en bibliothèque

- Fundamentals of chemical reaction engineering / Davis

Websites

- http://scgc.epfl.ch/telechargement_cours_chimie.htm