

ChE-403

**Heterogeneous reaction engineering**

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Cursus	Sem.	Type
Chemistry and Chemical Engineering		Obl.
Energy minor	H	Opt.
Ing.-chim.	MA1, MA3	Obl.

Language of teaching	English
Credits	4
Session	Winter
Semester	Fall
Exam	Written
Workload	120h
Weeks	14
<b>Hours</b>	<b>3 weekly</b>
Courses	2 weekly
Exercises	1 weekly
<b>Number of positions</b>	

**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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### 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:  $(\text{total points} \times 5 / 200 + 1)$ ; **the threshold is 111**.

For example:  $(111 \times 5 / 200 + 1) \# 4.0$

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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:  $(\text{points} \times 5 / 200 + 1)$ ; par exemple :  $(111 \times 5 / 200 + 1) \# 4.0$

### 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](#)

#### Références suggérées par la bibliothèque

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