



### 3.5. Chemical Reaction Engineering

**Course:**

Compulsory module for the master course Chemical and Energy Engineering

**Module:**

Chemical Reaction Engineering

**Objectives:**

Topic of the lecture Chemical Reaction Engineering is the quantitative assessment of chemical reactions, the selection of suitable reactor types and their design.

**Contents:**

1. Stoichiometry of chemical reactions
  - Key components and key reactions
  - Extent of reaction, conversion, selectivity and yield
2. Chemical thermodynamics
  - Reaction enthalpy
  - Temperature and pressure dependency
  - Chemical equilibrium
  - Free Gibbs enthalpy
  - Equilibrium constant  $K_p$  and temperature dependency
  - Pressure influence on chemical equilibrium
3. Kinetics
  - Reaction rate
  - Rate laws of simple reactions
  - Decomposition, parallel and series reactions
  - Equilibrium limited reactions
  - Estimation of kinetic parameters
  - Differential method
  - Integral method
  - Kinetics of heterogeneously catalyzed reactions
  - Adsorption and Chemisorptions
  - Langmuir-Hinshelwood kinetics
  - Temperature dependency of heterogeneously catalyzed reactions
4. Mass transfer in heterogeneous catalysis
  - Basics
  - Diffusion in porous systems
  - Pore diffusion and reaction
  - Film diffusion und reaction
  - Thiele module and pore efficiency factor
5. Design of chemical reactors
  - Reaction engineering principles
  - General mass balance
  - Isothermal reactors
  - Ideal batch reactor (BR)
  - Ideal plug flow tube reactor (PFTR)
  - Ideal continuous stirred tank reactor (CSTR)
  - Real technical reactors
  - Cascade of stirred tanks
6. Heat balance of chemical reactors
  - General heat balance
  - Cooled CSTR
  - Stability problems in chemical reactors
  - Residence time behavior
  - Calculation of conversion in real reactor systems



- Cascade model, Dispersions model, Segregation model
- Modeling of conventional fixed-bed reactors
- Selectivity problems
- Increase of selectivity in membrane reactors

7. Material aspects in chemical process engineering

- Importance of the chemical industry and feedstock
- Steam cracking of hydrocarbons
- Chemical products

**Teaching:**

Lecture, Tutorial; (summer semester); (2. semester of master studies)

**Prerequisites:**

**Workload:**

2 hours per week Lecture, 2 hours per week Tutorial, Lectures and tutorials: 56 hours, Private studies: 94 hours

**Examination/ Credits:**

written examination, 120 min, 5 CP

**Responsible lecturer:**

Prof. A. Seidel-Morgenstern, FVST, with Prof. Ch. Hamel as co-worker

**Literature:**

O. Levenspiel, Chemical Reaction Engineering, John Wiley & Sons, 1972