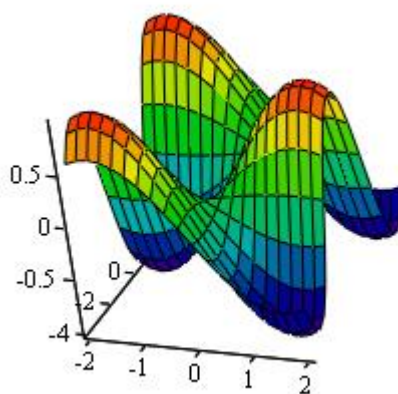


Computer-Aided Chemical Reaction Engineering

Datorberäkningar för industriella reaktorer



CACRE2018

28.5-5.6.2018

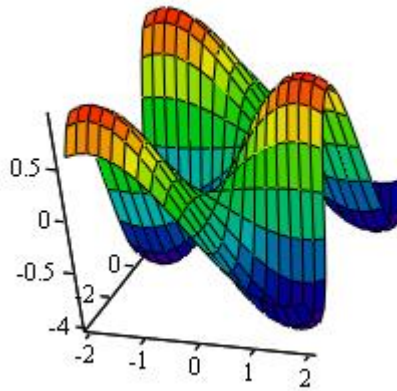
Axelia building, Seminar room Gadd, 1st floor
Biskopsgatan 8/Piispankatu 8, Turku/Åbo

Graduate School in Chemical Engineering (GSCE)
Åbo Akademi

A Course (8 cr, Bologna) 28.5-5.6.2018

Computer-Aided Chemical Reaction Engineering
Datorberäkningar för industriella reaktorer

CACRE 2018



Åbo Akademi, Axelia building, Seminar room Gadd
Biskopsgatan 8/Piispankatu 8, Turku/Åbo

Computer-Aided Chemical Reaction Engineering (CACRE2018)

Lecturers and demonstrators

Dr. Tapio Salmi, Professor, Åbo Akademi
Research interests: chemical reaction engineering

Dr. Heikki Haario, Professor, Lappeenranta University of Technology
Honorary guest lecturer
Research interests: numerical methods in science and engineering

Dr Dmitry Murzin, Professor, Åbo Akademi
Research interests: kinetics and catalysis

Dr. Johan Wärnå, Professor, Åbo Akademi
Research interests: modelling of chemical reactors

Dr Vincenzo Russo, Università di Napoli "Federico II"
Research interests: chemical reaction engineering and reactor modelling

Dr Teuvo Kilpiö, Researcher at Åbo Akademi
Research interests: multiphase reactor modelling

Dr Pasi Tolvanen, University teacher at Åbo Akademi
Research interests: process intensification

Dr. Cesar de Araujo Filho, Research scientist at AkzoNobel
Research interests: chemical reaction engineering and multiphase processes

Course material

will be distributed in the beginning of the course

Language

English

CACRE2018

Programme

Monday 28.5

9.15 -12.00

Basics of classical reactor modelling – homogeneous reactors
(Tapio Salmi)

12.00-13.15

Lunch

13.15-

Numerical methods for reactor modeling
Principles for construction of software
Exercises (Tapio Salmi, Johan Wärnä, Vincenzo Russo)

Tuesday 29.5

8.15-12.00

The role of molecular modeling in understanding catalytic processes
DFT in modeling of catalytic processes
(Dmitry Murzin)
Catalytic fixed bed reactors – models, algorithms and software
(Tapio Salmi, Vincenzo Russo)

12.00-13.15

Lunch

13.15-

Demonstrations and exercises
(Tapio Salmi, Johan Wärnä, Vincenzo Russo)

Wednesday 30.5

8.15-12.00

Catalytic fluidized beds –models and model solution strategies
Three-phase reactors – models for batch and continuous systems
(Tapio Salmi, Johan Wärnä, Vincenzo Russo)

12.00-13.15

Lunch

13.15-17.00

Exercises (Johan Wärnä, Vincenzo Russo)

Thursday 31.5

8.15-10.00

Transient reactor modelling
(Tapio Salmi, Teuvo Kilpiö)

10.15-12.00

Fluid-fluid reactors – models and solution strategies
(Tapio Salmi, Vincenzo Russo)

Exercises and demonstrations
(Johan Wärnä, Vincenzo Russo)

Friday 1.6

8.15-12.00

Fluid-solid reactions and reactors

(Tapio Salmi)

Micro- and millireactor technology

(Tapio Salmi, Teuvo Kilpiö, Vincenzo Russo)

12.00-13.15 Lunch

13.15-

Process intensification in reaction engineering: new reactors and methods (ultrasound, microwaves)

(Tapio Salmi, Pasi Tolvanen)

Exercises (Johan Wärnå, Vincenzo Russo)

Monday 4.6

8.15-12.00

Laboratory reactors and experiments in the collection of kinetic data; differential, integral and initial rate methods

(Tapio Salmi)

Principles of parameter estimation using nonlinear kinetic and reactor models

-algebraic, implicit algebraic and differential models- parameter estimation algorithms

(Tapio Salmi, Heikki Haario, Cesar de Araujo Filho, Johan Wärnå)

12.00-13.15 Lunch

13.15-

Presentation of a modeling tool (Teuvo Kilpiö)

Presentation of the exercises (Tapio Salmi, Johan Wärnå)

Parameter estimation starts (Heikki Haario, Johan Wärnå)

20.15- Social programme: dinner & random walk

Tuesday 5.6

9.15-12.00

Guest lecture of Dr Cesar de Araujo Filho (AkzoNobel): Chemical intermediates from glycerol – gas-liquid reactor technology from different perspectives

Guest lecture of N.N (to be confirmed)

12.00-13.15 Lunch

13.15-

Parameter estimation afternoon

Practical aspects and recent development in parameter estimation

- how to do the work in practice, sensitivities, contour plots, identifiability, Monte Carlo methods

(Johan Wärnå, Heikki Haario, Cesar de Araujo Filho)

17.00 Final conclusions