Course Package

Process Technology – Q1 +Q2

Name module	Process Technology – Q1 +Q2
Educational programme	MSc Chemical Science & Engineering
Period	First semester (quartile Q1 +Q2)
Study load	30 EC
Coordinator	C. C. Diepenmaat

Process Technology			
Quartile 1	**Quartile 2**	**Quartile 3**	**Quartile 4**
Chemical Reaction Engineering 201600218 (3,5 EC)	**Advanced Molecular Separations 201300049** (5 EC)		
Programming in Engineering 191158510 (1,5 EC)			
Advanced Chemical Reaction Engineering 201600151 (5 EC)			
Multi-component mass transport 201300050 (5 EC)			
Advanced Catalysis 201600152 (5 EC)	*Electrices: choose 5 EC*		
	Electrochemistry: Fundamentals& Techniques - 201800014 (5 EC)		
	Cost Management & Engineering -201400244 (5 EC)		
	Ion Transport in Fluids - 201800327 (2,5 EC)		

Required preliminary knowledge: To do this course package you need to have completed at least the first two years of your BSc. Equilibria; Physical Chemistry; Fluid Dynamics; Heat and Mass Transfer; Separation Technologies; chemical reaction engineering; Industrial Process; basic knowledge of catalysis and Kinetics.

Note: The required course is Chemical Reaction Eng. – 201600218 in order to be able to follow Advanced Chemical Reaction Engineering 201600151.

Quartile 1

201600218 - Chemical Reaction Engineering

The course starts with an introduction to ideal- (or model-) reactors (batch reactor, ideally mixed and plugflow reactor) and their characteristics. Setting up and solving the correct mass and energy balances plays a major role in the dimensioning of chemical reactors and is therefore a basic element of this course. With these balances, the degree of conversion, selectivity and yield for single and multiple reactions in single phase systems are calculated for stationary and instationary operation, for cascades of these modelreactors and for reaction systems of constant- and changing density. Subsequently the concept of Residence Time Distribution is introduced and used to describe non-ideal, intermediate states of mixing for continuous operated reactors, using both the tanks-in-series model and the plugflow-with-axial-dispersion model. The effects of micromixing (in addition to the macroscopic state of mixing discussed above) is discussed. The section on single phase reaction systems (and reactors) is concluded by analysing

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and solving problems related to combined heat effects with chemical reaction systems, especially in view of stable- and unstable operating points.

191158510 - Programming in Engineering

Computations are omnipresent in complex engineering problems in solid mechanics, fluid mechanics, civil and process engineering. Many problems are resolved with the aid of computers and dedicated programs today. Therefore, it is important for an engineer to be familiar with computers and programming languages. In this course, you will learn how to translate problems into algorithms and how to implement the algorithm into a computer language. We will focus on implementation in two widely used programming languages: Python or MATLAB, and C++. No previous programming knowledge is required. You will learn how to write, compile, and execute small programs in each language. We teach you how to write structured reusable code (object-oriented programming in Python and C++) and how to visualize your solutions (in MATLAB). Further, we teach how to better understand, analyze, optimise, and debug code.

201600152 - Advanced Catalysis

- Physisorption and capillary condensation for catalyst characterization
- Molecular bonding in chemisorption and heterogeneous catalysis on metals
- Oxide and solid acid catalysts
- Electro-photo- and plasma-catalysis
- Catalytst characterization with electrons and photons
- Temperature programmed techniques for characterization
- Catalytic reactors and transport

Quartile 2

201300049 - Advanced Molecular Separations

In Advanced Molecular Separations, separation technology is discussed starting from molecular properties up to full scale processes. The focus is on choosing a separation technology for given molecular properties, and the subsequent molecular design of more advanced separation technologies. For two separation technologies, fluid separations and membrane technology, the molecular design and separation process are treated in much greater detail, including a discussion on useful models to describe thermodynamics and mass transfer. The course will include two tests, one on fluid separations and one on barrier separations, but will also include two assignments on selecting the right separation technology for a given separation case.

Electives: choose 5 EC

201800014 - Electrochemistry: Fundamentals & Techniques

Electrochemistry deals with chemical changes caused by electricity (as in electrolyzers), and with the generation of electricity through chemical reactions (as in galvanic cells, i.e., batteries under discharge). Electrochemical processes are highly used in various branches of the industry and have an ever-increasing impact in our everyday life. Think, for example, of consumer products like batteries (e.g., in notebooks, smart phones or cars), electrosynthesis (or electrochemical conversion), electroplating or production of hydrogen by electrolysis of water. With more electrical energy being produced from solar and wind energy, a sustainable electricity supply will rely on storage. Additionally, aiming to phase out fossil-based fuels towards net zero carbon emission by 2050, the production of chemicals and fuels by alternative means will be required. Here, electrochemistry offers sustainable solutions, but further improvement of current and emerging electrochemical conversion techniques is needed.

The course consists of following activities:

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- Lectures and tutorials deal with the fundamental principles of electrochemistry, including thermodynamics, double layer structure, electrode reactions, and mass transfer in electrochemical systems. The main experimental techniques to study electrode reactions are also discussed

- The students carry out group practical projects and prepare a report discussing and interpreting the obtained results. The report is structured in the form of a research article. This allows students to familiarize with learned fundamentals and apply theoretical concepts to laboratory experiments and case studies in electrochemistry.

201400244 - **Cost Management and Engineering**

Course Objective:

The course objective is to provide engineering students with the theoretical understanding and practical approaches as well as the tools and techniques for the economic and financial evaluation of stand-alone but also competing design solutions for processes, products, construction projects, services and the practical application of the approaches in more complex settings. Engineers must be able to model the economic impacts of their recommendations during the life cycle of a project (widely interpreted). The course will focus on monetary quantification, using different system boundaries and perspectives. Students are challenged to go out and gather information on real-life applications of cost management and engineering techniques.

Teaching methods, assessment and language:

The course will use lectures and group assignments and self-study. The lectures will be a mix of instruction and some working on exercises. The students will also do independent research on subjects strictly related to the course. Subjects will be proposed in case students are at a loss about where to start, but it is strongly preferred that the students search a subject of their interest. This research activity takes place in a group and the group will write a report. The assessment and grading system will explained in more detail during the first lecture if necessary. By the way, the written examination consists of a mix of numerical questions and theoretical ones mainly related to the former. You may use a standard calculating device.

201800327 - Ion Transport in Fluids

Starting from the electrochemical potential, the Nernst-Planck equation will be derived and then used to understand the relative contribution of electromigration and diffusion. The validity of assuming electroneutrality in a fluid phase is discussed and investigated by introduction of the Poisson equation. In double layers and interfaces, the potential and ion distributions can be studied further. Next, the effect of fluid transport on ion transport and vice-versa will be introduced by combining the Poisson-Nernst-Planck equations with the Navier-Stokes equations. From this, electrokinetic mechanisms such as electro-osmosis can be derived. Finally, the use of these frameworks in relevant industrial procesess where ion transport plays a crucial role is explored.

Quartile Q1 & Q2

201600151 - Advanced Chemical Reaction Engineering

The course starts with a short overview/recap of required prior knowledge on single phase reaction systems. Subsequently, mass transfer models (film-, penetration- and surface renewal model) will be discussed and the effect of chemical reactions on the mass transfer rate is analysed in detail, both for homogeneous and heterogeneous reaction systems. Enhancement of mass transfer by chemical reactions during gas absorption, effectiveness factors for heterogeneous catalysts, selection of appropriate mass transfer models, analysis of kinetic rate data and reactor selection are elements discussed within the course. Fundamental mass transfer flux expressions (in general and for limiting situations) are derived, which can be used in multiphase reactor models. With this, reactor performance in terms of reactant conversion and product yield can be calculated, taking into account reaction kinetics and – equilibria, mixing (residence time distribution), multiple reactions (product selectivity) and heat effects.

201300050 - Multi-component mass transport

This course aims at understanding of mass transport in multi-component mixtures, based on a simplified version of the theory of Maxwell and Stefan.

Main aim is for students to be able to understand the basic principles of diffusion in mixtures containing various different species, driven by a combination of different driving forces, and to apply this understanding in specific relevant chemical technology applications.

Within the course a lot of attention is paid to contemplation and discussion, in order to consolidate the new knowledge and insights. Within this context, students are requested to give a lecture on one of the chapters in the book and to answer relevant case study, in which the multi-component characteristics of transport are evident. The case study involves the use, and stepwise extension, of an existing Matlab code, allowing the students to gradually and relatively independently simulate and study an eventually complex problem.

The course relies on prior knowledge from: Equilibria II, Fysical Chemistry, iFTV, FTV, Separation Technologies.

- The following topics are addressed:
- Limitations of the law of Fick;
- Driving forces for diffusion (potential gradients);
- Friction between molecules;
- Maxwell-Stefan (MS) concept;
- Bootstrap;
- Application of MS in relevant process (membranes, heterogeneous catalysis, transport at interfaces);
- Extending Matlab code for relatively complex simulations.

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