Monday (October 3, 2016)

Lecture 1: Introduction to catalysis & self-assembly

By Dr. Evgeny Pidko and Dr. Marijn van Huis

ABSTRACT

Introduction to Catalysis (Evgeny Pidko)

In this section I will present a general introduction to the Catalysis Science and Technology with the main emphasis of the fundamental physical-chemical concepts and inorganic chemistry of catalysis. The lecture will start with a recap of the key concepts of catalysis such as the definitions and classifications and the role of catalysis for the humanity. Next, by using a relevant recent example from catalytic chemistry of carbon dioxide, I will introduce the fundamental concepts of potential energy surface and reaction mechanisms and discuss what fundamental properties are needed to make a catalytic system successful. Here, the key parameters such as activity, selectivity and lifetime and their relations with the mechanism and energetics of a catalytic reactions will be introduced. Examples from both homogeneous and heterogeneous catalysis will be given to highlight the common inorganic chemistry and outline the main principles that one may follow when selecting one or another for a given application.

Quantitative Imaging of Self-Assembled Nanostructures for Catalysis (Marijn van Huis)

The properties and performance of nanostructured materials depend greatly on the way they are arranged and ordered. Detailed studies on the 3D distribution of catalytic nanoparticles in porous supports such as zeolites have provided insight into the collective catalytic properties of nanostructured materials. Instead of growing the catalytic nanoparticles more or less randomly onto supports, self-assembly (SA) approaches can be used to build superstructures of ordered nanoparticles, such as 2D arrays of nanoparticles that self-assemble at liquid-liquid or liquid-gas interfaces, and 'supraballs' wherein nanoparticles are ordered in 3D arrangements. New material properties can emerge from the combinations of different kinds of nanoparticles, e.g. by combining metallic, metal oxide, and semiconductor nanoparticles. To determine the structure of these novel materials and to establish structure-property relationships, proper characterization methods are key. In this section I will address experimental methods to determine quantitatively the 3D structure of (assembled) nanostructural materials. In particular electron tomography, X-ray tomography, 3D reconstruction algortihms, advanced data processing, and simulation tools will be discussed.

Lecture 2: Introduction to fluidics

By Prof. Detlef Lohse and Prof. Todd Squires *(University of California, Santa Barbara)*

ABSTRACT

Surface nanobubbles and nanodroplets (Detlef Lohse)
Surface nanobubbles are nanoscopic gaseous domains on immersed substrates which can survive for days. They form whenever local gas oversaturation occurs, be at through chemical reactions, electrolysis, or through solvent exchange. I will give an overview on surface nanobubbles, but also on surface nanodroplets, which are nanoscopic droplets (e.g. of oil) on (hydrophobic) substrates immersed in water, as they show very similar properties and can easily be confused with surface nanobubbles and as they are produced in a very similar way, namely by a solvent exchange process, leading to local oversaturation of the water with gas or oil, respectively, and thus to nucleation.

I will briefly report how surface nanobubbles and nanodroplets can be made, how they can be observed (both individually and collectively), and what their properties are. I will then explain the long lifetime of the surface nanobubbles. The crucial element is pinning of the three-phase contact line at chemical or geometric surface heterogeneities. The dynamical evolution of the surface nanobubbles then follows from the diffusion equation, Laplace's equation, and Henry's law. In particular, one obtains stable surface nanobubbles when the gas influx from the gas-oversaturated water and the outflux due to Laplace pressure balance. This is only possible for small enough surface bubbles. It is therefore the gas oversaturation ζ which determines the contact angle of the surface nanobubble or nanodroplet and not the Young equation.
The talk reports on joint work with Xuehua Zhang and several postdocs and PhD students.

Lecture 3: Introduction to chemical reaction engineering

By Prof. Hans Kuipers

ABSTRACT

Introduction to Chemical Reaction Engineering
In this session a general introduction to Chemical Reaction Engineering (CRE) will be presented with emphasis on the design and operation of chemical reactors. In the first lecture we will focus on single phase chemical reactors whereas in the second lecture we will focus on multiphase chemical reactors.

Single Phase Chemical Reactors (45 min)
In the first lecture the basic concepts (conversion, selectivity and yield) will be introduced together with a discussion of the main types of model reactors and the associated mathematical description and design procedures. Subsequently the representation of non-ideal flow will be introduced together with short-cut methods facilitating the rational design of single phase chemical reactors exhibiting non-ideal flow behavior. Finally the thermal behavior of single phase chemical reactors will be briefly discussed.

Multi-Phase Chemical Reactors (45 min)
In the second lecture an introduction to the field of multiphase chemical reactors will be presented: the main reactor types and the flow regimes will be discussed as well as the associated key phenomena/models relevant for design/scale-up and operation of these reactors. Specific attention will be paid to the mass and heat transport phenomena prevailing in these reactors. Finally future challenges will be highlighted to improve the design and scale-up procedures and (ultimately) the performance of multiphase chemical reactors.

Invited lecture A: Energy challenge

By Prof. Gert Jan Kramer *(Copernicus Institute, Utrecht University)*

ABSTRACT

The Energy Challenge
The societal challenge and the evolving engineering challenges

Over the past decade the “energy challenge” has come in ever sharper focus: the world needs to transform its energy system from one that has for over a century been dominated by (fossil) hydrocarbons, to one that is dominated by electric renewables with hydrocarbons in a support role. We know that it is technically possible; we just don’t know if we can deliver it. This is the societal challenge.

Simultaneously, while this transition unfolds, the world will see a move away from molecular energy delivery with catalysis and processes engineering as dominant disciplines supporting it, to a world in which energy delivery is primarily through “devices and electrons” with electrical engineering, IT and materials as key supporting disciplines.

Still… plenty of challenges remain and new ones develop in the realms of catalysis and chemical engineering.

Tuesday (October 4, 2016)

Invited lecture B: Fluidics

By Prof. Todd Squires *(University of California, Santa Barbara)*

ABSTRACT

Coupling heat, mass, and fluids in reacting systems
We will describe paradigmatic problems that involve the coupling between mass transport, heat transfer, and fluid flows. Such problems arise in a wide variety of natural, biological, industrial, and technological systems. We will motivate and describe dimensionless parameters, which are often fairly easy to estimate for experimental systems, and which give strong qualitative intuition for how a system behaves. We will explore subtle ways in which mass transport is coupled with fluid flows, and vice versa, and how those can influence reacting systems more generally.

Wednesday (October 5, 2016)

Invited lecture C: Catalysis / self-assembly

By Prof. Eelco Vogt *(Albemarle, part-time professor Utrecht University)*

ABSTRACT

Catalysis in real life
Catalysis is big business. It takes place in huge refinery reactors that are several stories high, and treats millions of barrels of feedstock each day to make our transportation fuels, polymers for clothing and other applications, and our food. How do we translate the fundamental chemistry that takes place on a molecular scale at surface and interfaces into these industrial processes? What hurdles do we encounter when going from atoms to tons, and how do we solve them?

Thursday (October 6, 2016)

Lecture 4: Probing catalysts with molecular experimentation techniques

By: Dr. Jovana Zecevic and Dr. Joel Schmidt (UU)

ABSTRACT

Probing catalysts with molecular experimentation techniques
As catalysts facilitate chemical bond formation and destruction, it is vital that the composition and activity of these micrometer particles is thoroughly understood. To this end, experimental probing techniques are required at different length-scales. On the nanoscale, Transmission Electron Microscopy (TEM), is an important technique that can provide morphological information such as shape, porosity, structural integrity. At the atomic scale, spectroscopic techniques are used that study the materials using electromagnetic radiation, which can probe local chemical environment. These reliably give insight into materials, and can also be applied in-situ to study catalysts under realistic operating conditions, so that their true nature "in action" can be understood.

Lecture 5: Mesoscale particle-based & continuum modelling

By: Dr. Johan Padding

ABSTRACT

In two lectures (2x50 minutes) I will present the basics of modern computational methods that can capture flow and diffusion in solid-liquid and solid-gas systems. Understanding flow and diffusion of such systems at mesoscales, i.e. at scales which are much larger than the molecular scale, but still much smaller than the reactor scale, is very important for optimizing reactors and energy conversion systems based on flow.
I will first introduce the principles behind coarse-grained mesoscale particle-based methods, which explicitly obey the laws of conservation of mass and momentum, where the transport coefficients appear from the coarse-grained interactions. These methods are ideal for scales at which both flow and detailed Brownian motion of particles are important. Two explicit examples, Dissipative Particle Dynamics and Multi-Particle Collision Dynamics, will be treated in more detail.
Then I will introduce continuum methods, where the transport coefficients are input instead of output. These methods are ideal for scales at which Brownian motion of particles can be captured by a Fickian or equivalent equation.

Topics include:

- General principles of particle-based simulations
    - Forces on particles
    - Neighbourlists
    - Numerically integrating Newton's equations of motion
- Coarse graining and hydrodynamic interactions
- Brownian motion of a single particle
- Overview of mesoscale methods with hydrodynamic interactions
- Dissipative Particle Dynamics
- Multi-particle Collision Dynamics
- Application: dynamics of colloidal suspensions
- General principles of continuum methods
    - Navier-Stokes and Fick equations
    - Discretizing the equations
    - Solution methods
- Application: flow and diffusion past a sphere with reactive surface

Friday (October 7, 2016)

Lecture 6: Quantum-chemical & molecular modelling

By: Dr. Ivo Filot

ABSTRACT

Advances in simulation methodology and the rise in computing power have resulted in a wide variety of computational methods applicable to the field of catalysis. When several such methods are combined, catalytic phenomena of increasing complexity can be studied by computational means. The connection between density functional theory calculations and microkinetics simulations is such a multiscale approach; it provides an essential tool to develop an atomistic understanding of catalytic performance. In this approach, the molecular properties such as electronic energies are bridged with macroscale properties such as reaction kinetics. In this presentation, it will be show how DFT-based kinetic parameters can be used in microkinetics models that are able to elucidate mesoscale phenomena in catalysis.

Lecture 7: Mesoscale experimental techniques

By: Prof. Michel Versluis (UT) en Prof. Niels Deen

ABSTRACT

In chemical processes, knowledge of local conditions is crucial in order to understand and optimized the process performance. Most specifically, one would be interested in distribution of pressure (p), temperature (T), concentration (c), and velocity (u). Besides, it is important to gain information regarding length scales that are present in the heterogeneous system, e.g. bubble (droplet, particle) size.
In this course, an overview will be presented regarding the methods to obtain information regarding characteristic length scales and the mentioned scalars p, T, c, and vector u. These experimental techniques can be either invasive or non-invasive.