MONDAY (October 12, 2015)

	Foyer	*Plenary hall*	*Free area*	*Grand Cafe*	*Comments*
8.30-9.00	Welcome				
9.00-9.45		**Session 1**			
9.45-10.00	Break	**By:** Bert Weckhuysen and Hans Kuipers			
10.00-10.45		**Title:** Energy Challenge: From Single Molecule to Reactor			
10.45-11.00	Break				
11.00-11.45		**Session 2**			
11.45-12.00	Break	**By:** Bert Weckhuysen			
12.00-12.45		**Title:** Heterogeneous Catalysis: Principles and Practice (including explanation case study)			
12.45-13.45	Lunch				
13.45-14.30		**Session 3**			
14.30-14.45	Break	**By:** Rutger van Santen			
14.45-15.30		**Title:** Concepts of Heterogeneous Catalysis			
15.30-17.00			Meet & Greet with the tutors Teamwork: case study		Meet with the tutors (Rosa Bulo, Johan Padding, Rob Lammertink)
17.00-19.00		***Discussion/workshop: How to succeed your PhD in a multicultural team***			
19.00-20.30	Diner				
20.30-				Scientific discussions at the bar	

MCEC School Program

MONDAY

Session 1
By: Bert Weckhuysen and Hans Kuipers
Title: Energy Challenge: From Single Molecule to Reactor

This course module starts with a basic introduction on catalysis, with some historic reflections, including the role catalytic materials have in contributing to the energy challenge. In a next step, it will be demonstrated that catalysis is a truly multi-scale science and you can join a journey through space and time in which we will travel through the reactors and piping of a chemical factory in which a particular catalyst material is applied. With a Google Earth-like camera, we can zoom in from the reactor scale to the nanoscale and see what exactly happens on the level of one catalyst particle, one atom and even one molecule. The aspects of intra- and interparticle heterogeneities will be introduced. This talk will end with the introduction of reactor aspects, including reactor types, heat and mass flow aspects as well as catalyst regeneration.

Session 2
By: Bert Weckhuysen
Title: Heterogeneous Catalysis: Principles and Practice

Although many people have no idea of the existence of catalysis, their daily life is based on it. Catalysts are used in the production of the foods that we eat, the clothes that we wear, the energy necessary to heat and cool our homes, the processes that occur throughout our body to provide function to nearly every organ, the purification of the air that we breathe, the production of the fuels used in our cars, trucks and planes, and the manufacturing of the materials, such as plastics, used in and around our homes and offices. In this course module the fundamental principles and practice of heterogeneous catalysts will be introduced. As an example, we will discuss in detail the Fluid Catalytic Cracking (FCC) process, heavily used for the production of transportation fuels, namely gasoline, and key chemical building blocks, in particularly propene, from crude oil fractions. By taking this showcase, the principles of catalyst activity, selectivity and stability will be highlighted, as well as the concepts of zeolite chemistry and catalysis will be introduced.

Session 3
By: Rutger van Santen
Title: Concepts of Heterogeneous Catalysis

Catalyst performance depends on activity, selectivity and stability. The relation between catalyst performance and its structure and composition is essential to understand. The physicochemical phenomena that are responsible will vary with the choice of reaction, catalyst and process conditions. The description of the catalytic reaction requires a mechanistic model so that the corresponding catalytic reaction cycle can be constructed. Explicit knowledge has to be available on the relation between the state of the catalysts surface and elementary rate constants. Such data have to be provided by experiment and are also more and more provided by computation. It provides input to a (micro) kinetics model that with the available tools of current computational catalysis can be used to predict catalyst performance optimization parameters. In this course module the required background will be provided to understand the main concepts of heterogeneous catalysis. This will be done by discussing the following showcase studies, which provide a representative overview of different catalytic system properties:

- ¾ Transition metal-catalyzed CO conversion: This reaction demonstrates the relevance of knowing relative reaction rate parameters and mechanism. Also catalyst activation will be discussed.
- ¾ Zeolite-catalyzed hydrocracking: This reaction illustrates the need to know adsorption equilibria of complex mixtures in its micropores. It also illustrates a stability principle. It allows also comparing the principles of hydrocracking and fluid catalytic cracking processes.
- ¾ Selective oxidation of ethylene: This example shows that selectivity varies with the state of the catalyst surface.
- ¾ Oxygen evolution reaction and photo catalysis: Here will be system integration and structure dependency discussed.

TUESDAY (October 13, 2015)

	Foyer	*Plenary hall*	*Free area*	*Grand Cafe*	*Outdoor*	*Comments*
8.00-8.30	Welcome					
8.30-9.15		**Session 4**				
9.15-9.30	Break	**By:** Bert Weckhuysen and Albert van den Berg				
9.30-10.15		**Title:** Microreactors, Microfluidics and Analytical Methods				
10.15-10.30	Break					
10.30-14.00					**Outdoor activity: Teamgame (including lunch)**	Organised by Team Community & Communication (Mathieu Odijk, Miguel Solsona, Ivan Devic, Lennart Weber)
14.00-14.45		**Session 5**				
14.45-15.00	Break	**By:** Marjolein Dijkstra and Alfons van Blaaderen				
15.00-15.45		**Title:** Multiscale Structuring by Hierarchical Self-Assembly: Experiments, Simulations & Theory				
15.45-16.00	Break					
16.00-16.45		**Session 6**				
16.45-17.00	Break	**By:** Marjolein Dijkstra and Alfons van Blaaderen				
17.00-17.45		**Title:** Multiscale Structuring by Hierarchical Self-Assembly: Experiments, Simulations & Theory				
17.45-19.00			Teamwork: case study			
19.00-20.30	Diner					
20.30-				Scientific discussions at the bar		

MCEC School Program

TUESDAY

Session 4
By: Bert Weckhuysen and Albert van den Berg
Title: Microreactors, Microfluidics and Analytical Methods

In this course module, an introduction of the microreactor concept will be given, with attention to their advantages, challenges and opportunities. Various microfluidic technologies and methods will be presented and their importance to the realization of microreactor devices will be given. The advantages or different fabrication techniques and materials as well as needed infrastructure will be presented. Besides the possibilities for chemical production using the “numbering up” principle, most emphasis will be laid on the possibility to integrate sensing and analytical methods. Apart from integrated electrochemical and optical sensing, impedance spectroscopy, mass spectrometry and Surface Enhanced Raman Spectroscopy (SERS) will be discussed. Special attention will be paid to the introduction of optical spectroscopic techniques, which could be directly coupled to catalytic reactor set-ups in which literally the spectrometer is brought to the reactor. These methods include optical fiber technologies (e.g. UV-Vis and Raman probes) as well as insertion technology (e.g. ATR-IR devices), allowing focusing on the consumption or formation of reactants, reaction intermediates and reaction products, as well as on the state of the (active) catalyst material. Illustrative key results will be presented revealing the current state-of-the-art of the methods, including a discussion on their possibilities and limitations, together with the future challenges.

Session 5
By: Marjolein Dijkstra and Alfons van Blaaderen
Title: Multiscale Structuring by Hierarchical Self-Assembly: Experiments, Simulations & Theory

In this course module we want to give an impression of what is necessary both experimentally, but also through input of simulations and theory to arrive at multiscale structures that are going to be used in MCEC projects and for other research in the field of energy conversions. We will focus the multi-step Self-Assembly (SA) of colloidal particles, starting form structuring nanoparticles, and going up in length scales from these, but the methodology is applicable also to other cases (e.g. using molecular or supramolecular building blocks). After explaining how colloidal matter is different from other forms of matter, but still is able to form equilibrium phases, we will give illustrative examples of (nano-) particles: the first building blocks. Subsequently, the way such particles interact (through Van der Waals forces, steric, depletion and double layer overlap forces) will be qualitatively treated. Also several examples are given of the state of the art to measure forces between colloids. Determining these interactions is quite important as they determine the equilibrium phase behavior, which can be investigated quite effectively also by a combination of computer simulations (more detailed below) and theory.

Session 6
By: Marjolein Dijkstra and Alfons van Blaaderen
Title: Multiscale Structuring by Hierarchical Self-Assembly: Experiments, Simulations & Theory

If structures are made by Self-Assembly (SA), which goes too fast, kinetic pathways and traps like glassy states become important as well. In the case of out-of-equilibrium SA also the role of hydrodynamics does become important and does not drop out like it does for an equilibrium pathway. Next in this course module, the methodology will be discussed on how SA can be manipulated and stirred into desired directions, e.g. by the use of several (and even combinations of) external fields, like electric fields (including optical fields such as in optical tweezers), magnetic fields, gravitational field, shear (liquid flow), structured walls and confinement. Pathways that will be used in the MCEC program to perform SA in stages will be briefly mentioned as well. The various techniques that are used to study SA or self-organization processes of (colloidal) particles in computer and that can be used to predict the crystal structures of these systems and to map out phase diagrams are: Monte Carlo simulations, Brownian Dynamics simulations, Molecular Dynamics simulations, Stochastic Rotation Dynamics. We will show examples for binary nanoparticle superlattices, rod-like and plate-like particles and how differences in shape and potential affect the structures.

WEDNESDAY (October 14, 2015)

	Foyer	*Plenary hall*	*Free area*	*Grand Cafe*	*Outdoor*	*Comments*
8.00-8.30	Welcome					
8.30-9.15		**Session 7**				
9.15-9.30	Break	**By:** Detlef Lohse				
9.30-10.15		**Title:** Introduction to Single-phase Flow				
10.15-10.30	Break					
10.30-11.15		**Session 8**				
11.15-11.30	Break	**By:** Hans Kuipers and Detlef Lohse				
11.30-12.15		**Title:** Introduction to Multiphase Flow and Multiphase Chemical Reactors				
12.15-13.15	Lunch					
13.15-14.00		**Session 9**				
14.00-14.15	Break	**By:** Hans Kuipers and Niels Deen				
14.15-15.00		**Title:** Experimental and Computational Techniques for Multiphase Flows				
15.00-15.30	Break					
15.30-17.30					**Outdoor activity: Teambuilding and communication**	Organised by Relais Outdoor
17.30-18.00	Break					
18.00-19.00	Diner					
19.00			Teamwork: case study	Scientific discussions at the bar		

MCEC School Program

WEDNESDAY

Session 7
By: Detlef Lohse
Title: Introduction to Single-phase Flow

In this course module a general introduction to single-phase flow will be presented with emphasis on dimensional analysis, dimensionless groups and the theoretical framework describing flow and scalar transport in single-phase systems. The Navier-Stokes equations will be introduced and discussed together with the conservation equations for scalar transport (i.e. mass and heat conservation equations). Finally future challenges will be highlighted such as the treatment of turbulence.

Session 8
By: Hans Kuipers and Detlef Lohse
Title: Introduction to Multiphase Flow and Multiphase Chemical Reactors

In this course module an introduction will be presented to the field of multiphase flow and multiphase chemical reactor engineering. Following a classification of multiphase flows the session will focus on dispersed multiphase flows with emphasis on the theoretical framework to describe these flows. Both the behavior of individual dispersed elements (bubbles, drops or particles) as well as the collective behavior of dispersed flows will be discussed including the role of turbulence. Subsequently an introduction to the field of multiphase chemical reactors will be presented: the main 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.

Session 9
By: Hans Kuipers and Niels Deen
Title: Experimental and Computational Techniques for Multiphase Flows

In this course module an overview of the different computational and experimental techniques available for multiphase flows will be presented and discussed. Popular non-invasive monitoring techniques will be presented and discussed as well as (multi-scale) computational techniques for dispersed multiphase flows. Illustrative key results will be presented revealing the current state-of-the-art of the computational and experimental techniques. Possibilities and limitations of these techniques will be highlighted together with the main future challenges.

THURSDAY (October 15, 2015)

	Foyer	*Plenary hall*	*Sub hall*	*Free area*	*Grand Cafe*	*Comments*
8.00-8.30	Welcome					
8.30-10.00		**Plenary session: Solar Fuels** **By:** Prof. Thomas F. Jaramillo (Stanford University, Invited speaker) **Title:** Generating fuels from sunlight: Catalyst design, development, and integration into devices				
10.00-10.15	Break					
10.15-13.00		**Parallel session Biomass** **By:** Dr.ir. Ruud van Ommen (Delft University of Technology, Invited speaker) **Title:** Introduction to Biomass Conversion and **By:** Pieter Bruijnincx **Title:** Biomass research within MCEC	**Parallel session Solar Fuels** **By:** Monica Barroso **Title:** Scientific and technological challenges in solar fuels research			
13.00-14.00	Lunch					
14.00-15.30		***Discussion/workshop: How to build MCEC Community***				Organised by Mathieu Odijk and Emke Molnar
15.30-18.30				Teamwork: case study		
18.30-19.30	Diner					
19.30-				Teamwork: case study	Scientific discussions at the bar	

MCEC School Program

THURSDAY

Plenary Session
By: Prof. Thomas F. Jaramillo (Stanford University, Invited speaker) http://jaramillogroup.stanford.edu/tom.html
Title: Generating fuels from sunlight: Catalyst design, development, and integration into devices

Tentative abstract:
"Utilizing solar energy to drive chemical transformations is a promising means for the renewable, sustainable production of large-scale fuels and chemicals while minimizing the use of fossil resources. Examples include solar photoelectrochemical (PEC) water-splitting as well as water and/or CO2 electrolyzers coupled to solar photovoltaics. Catalyst development is crucial in these areas, notably to drive reactions such as the hydrogen evolution reaction (HER), the oxygen evolution reaction (OER), and the CO2 reduction reaction (CO2RR). This presentation will cover challenges and opportunities involving the development of catalysts for these reactions, as well as their integration into devices such as semiconductor photoelectrodes and water electrolyzers."

Parallel Session Biomass
By: Dr.ir. Ruud van Ommen (Delft University of Technology, Invited speaker) http://cheme.nl/ppe/people/vanommen.shtml
Title: Introduction to Biomass Conversion

By: Pieter Bruijnincx
Title: Biomass research within MCEC

Ruud van Ommen will introduce e.g. socioeconomic aspects of Biomass Conversion along with specific subjects in biomass research as biomass composition, properties and characterization. Pieter Bruijnincx will discuss biomass research that is directly related to the MCEC program.

Parallel Session Solar Fuel

By: Monica Barroso

Title: Scientific and technological challenges in solar fuels research

This tutorial session will be focused on the key challenges currently faced in the context of solar fuels synthesis, and possible strategies to overcome these barriers. From the development of new materials (light-absorbers, catalysts) to new device architectures, we will discuss the current state-of-the-art in the field of solar water splitting and CO_2 reduction, identify the main challenges and limitations of the existing systems, and explore new approaches to achieve the “holy grail” of clean and renewable energy.

FRIDAY (October 16, 2015)

	Foyer	*Plenary hall*	*Free area*	*Grand Cafe*	*Comments*
8.30-10.00		Teamwork: case study	Teamwork: case study	Teamwork: case study	
10.00-10.15	Break				
10.15-13.00		**Plenary session** **By:** Krijn de Jong and Emiel Hensen **Title:** Synthesis gas production and conversion – from fundamentals to commercial application			
13.00-14.00	Lunch				
14.00-16.00		**Presentations: Case Sudies**			
16.00-	Goodbye				

MCEC School Program

FRIDAY

Plenary Session
By: Krijn de Jong and Emiel Hensen
Title: Synthesis gas production and conversion – from fundamentals to commercial application

In this session we intend to present and discuss the science and technology related to synthesis gas, a mixture of CO and H2 that can be produced from any carbon containing feedstock. First the production of synthesis gas will be introduced by Prof. Emiel Hensen. Second Prof Krijn de Jong will discuss Gas to Liquids technology at all relevant length scales (nm to km). Third, Prof. Emiel Hensen will present the fundamentals of the metal catalyzed conversion of synthesis gas to hydrocarbons also known as the Fischer Tropsch Synthesis.