12 June - Shell visit

09.30 - 10.00	Registration + placing poster on poster boards
10.00 - 10.30	Introductory talk Evren Ünsal
10.30 - 12.00	Tours through the labs
12.00 – 13.30	Lunch and poster sessions
13.30 – 14.00	Presentation; Chemical processes within Shell by Sipke Wadman
14.00 - 14.30	Presentation; Carbonates by TBD
14.30 – 15.00	Talk by Sanjana Chandrashekar
15.00 – 15.30	Break
15.30 – 17.00	ETCA
16.00 – 17.00	Energy Transition Game
17.00 – 17.30	Lecture Energy Storage by Peter Klusener
17.30 – 18.30	Pont to Restaurant Pllek
18.30 – 21.00	Drinks and dinner
21.00	Bus to Hotel van der Valk, Dordrecht

13 June – Hotel vd Valk te Dordrecht

09.00 – 09.45	The electrification of chemical conversion processes by means of plasma-assisted non-thermal processes by Prof.dr.ir. M.C.M. van de Sanden (Richard)
09.45 – 10.30	Science speed dating (3 x 15’)
10.30 – 11.00	Break
11.00 – 12.00	WELCOME TO OUR LABS: *about techniques and equipment* Ali Fathiganjehlou (TU/e), Sofie Ferwerda (UU) and Andries Jensma (RUG)
12.00 – 13.00	Lunch
13.00 - 13.45	(Machine) Learning What Makes Catalysts Good by Dr. Nong Artrith
13.45 – 15.00	A radical green chemistry transition? By Prof.dr. Derk. A. Loorbach
15.00 - 15.30	Break
15.30 – 16.15	Membranes and Membrane reactors for process intensification by Prof.dr. F. (Fausto) Gallucci
16.15 – 21.30	Social Activities and dinner

14 June – Visit Shell Moerdijk

08.00 – 09.00	Bus to Moerdijk
09.00	Registration, safety, briefing and intro site Introduction Shell Chemie; What are our plans to the future? Coffee / break Shell Moerdijk Strategy Lunch, and safety clothes Outside: Factory specific information (detailed information about the process + latest safety briefing) Factory tour through the relevant units Bicycle tour over Moerdijk site
15.30	End program - Bus to station Dordrecht CS

Abstracts

Derk Loorbach

Title: A radical green chemistry transition?

Abstract: In this interactive lecture, prof. Loorbach will introduce the transition perspective and how transformative research can contribute to achieving just and sustainable futures. Whereas most policies have been led for decades by engineers and economists to generate growth and innovation, we are increasingly facing the negative consequences. Ecological collapse and growing social inequalities are threatening future stability, but so far keep being addressed by the same recipe that created the problems. What we need, argue transition researchers, is a value-based and design oriented process of radical and systemic social change (transition), which by definition will not come from optimizing what is already there but is in essence a process of destruction, phase-out, adaptation and build-up in one. Navigating such a process is in essence an action research project at a societal level: we need to reinvent an economy and industry that is without emissions, waste and thus sustainable and linear. The best possibility to achieve this would imply things like a radical decrease in resource consumption, circular production and a shift to renewables. This is politically and socially challenging: vested interests and locked-in policies and institutions resist such changes to prioritize incremental, gradual innovation. In this session we will discuss what the transition perspective means for fundamental research. How to embed in in a desired transition? How to prevent hijacking or greenwashing? How to develop the right coalitions? Ho to collaborate across disciplines towards transition?

Richard van de Sanden

Title: The electrification of chemical conversion processes by means of plasma-assisted non-thermal processes

Abstract: In this present I will give an overview of the status of chemical conversion processes by means of plasma-assisted non-thermal processes. In particular I will focus on the cases of non-thermal plasma conversion of CO_2, N_2/O_2 and CH_4 using microwave generated plasmas. The background is renewable energy driving chemistry in which the non-thermal properties of plasma (difference in temperatures between the electrons, the molecules and their vibrational degrees of freedom), possibly with the assistance of catalysts, can drive chemical conversions beyond the thermodynamic limit. Important aspects as energy and conversion efficiency and the underlying non-thermal chemistry and kinetics at play, as determined using several (in situ) diagnostics will be highlighted. In addition, some novel approaches in which plasma are combined with electrochemical conversion using hydrogen or oxygen transporting membranes and their potential advantages, will be discussed.

Nong Artrith, N. (Nong)

Title: (Machine) Learning What Makes Catalysts Good

Abstract: Machine learning (ML) has proven a powerful tool for accelerating the computational characterization of energy materials. There is a growing number of case studies identifying descriptors of catalytic performance using ML instead of physical intuition. ML is ideally suited for the pattern detection in large uniform data sets, but consistent experimental data sets on catalyst studies are often small. Here we demonstrate how a combination of machine learning and first-principles calculations can be used to extract knowledge from a relatively small set of experimental data. The approach is based on combining acomplex machine-learning model trained on a computational library of transition-state energies with simple linear regression models of experimental catalytic activities and selectivities from the literature. Using the combined model, we identify the key C-C bond-scission reactions involved in ethanol reforming and perform a computational screening for ethanol reforming on monolayer bimetallic catalysts. The model also predicts four promising catalyst compositions for future experimental studies. The approach is not limited to ethanol reforming but is of general use for the interpretation of experimental observations as well as for the computational discovery of catalytic materials.

Fausto Gallucci

Title: Membranes and Membrane reactors for process intensification

There is general consensus on the contribution that process intensification can give to the chemical industry in terms of improced energy efficiency. In general, Process Intensification (PI), is defined as “any chemical engineering development that leads to a substantially smaller, cleaner, safer and more energy efficient technology” (Reay et al., 2013), and is always referred to as the next revolution of the chemical industry.

One interesting strategy is achieved in the synergy domains, where functions are integrated in single units. Generally, the functions integrated are reaction and separation or reaction and heat management. The integration of functions promises to decrease the capital costs and operating costs compared to typical systems where these functions are separated.

One of these “novel” concepts is the membrane reactor concept, in which membrane separation is integrated with reaction.

This talk summarizes the work on membrane reactors for a variety of applications and integration of membrane reactors with different concepts.