Annual Report 2009

KinCat
Strong Point Centre Kinetics and Catalysis

The centre was established July 1, 1998 by NTNU and SINTEF in recognition of the strong scientific level of the members participating. The centre consists of the catalysis group, Department of Chemical Engineering, NTNU and the catalysis research team, SINTEF Materials and Chemistry. As of January 2008 the centre has been established as a Gemini centre by NTNU and SINTEF.

Program leader:

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This report was edited by:

Karin Wiggen Dragsten
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Annual Report 2009

KINCAT

Strong Point Centre Kinetics and Catalysis

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KinCat Members Spring 2010

Department of Chemical Engineering
Group for Petrochemistry and Catalysis

Academic staff

Professor Edd A. Blekkan
Professor De Chen
Professor Anders Holmen
Professor Magnus Rønning
Assoc. professor Hilde J. Venvik
Adjunct professor Erling Rytter
Adjunct professor Kjell Moljord

Laboratory personel

Engineer Karin Wiggen Dragsten

Doctoral students

Hamidreza Bakhtiary
Anh Hoang Dam
Hassan Dar
Asmira Delic
Sara Boullosa Eiras
Ilya Gorelkin
Daham Gunawardana
Fatemeh Hayer
Fan Huang
Saima Sultana Kazi
Oana Mihai
Navaneethan Muthuswany
Tayyaba Noor
Eleni Patanou
Xuyen Kim Phan
Paul Radstake
Shreyas Rane
Miroslav Surma
Ingvild Tronstad
Nikolaos Tsakoumis
Charita Udani
Nicla Vicinanza
Alexey Voronov
Jia Yang

Postdoctoral fellows 2009/2010

Nina Hammer
Estelle Vanhaecke
Bjørn Christian Enger
He Li
Tiejun Zhao
Jun Zhu
Hongmin Wang
Espen Wangen
Ingeborg_Helene Svenum

Guests 2009

Christine Balonek, (PhD. student, UMN, Minneapolis, USA)
Wayne Blaylock, (PhD.student, MIT, Boston, USA)
Sara Lögdberg (Ph.D. student, KTH, Stockholm, Sweden)
Fernando Bimbela (Ph.D. student, University of Zaragoza, Spain)

Technical and administrative staff shared with other groups at the Department of Chemical Engineering

Harry T. Brun
Arne Fossum
Jan-Morten Roel
Lisbeth H. B. Roel

SINTEF Materials and Chemistry, Catalysis and Kinetics

Administration

Research Manager Torbjørn Gjervan
Senior-/Project Secretary Berit Broli

Research scientists
Research Scientist Håkon Bergem
Research Scientist Svatopluk Chytil
Research Scientist Ingvar Kvande
Research Scientist Anna Lind
Research Scientist Odd Asbjørn Lindvåg
Research Scientist Hilde Meland
Research Scientist Rune Myrstad
Senior Scientist Rune Lødeng
Professor II Emeritus Odd A. Rokstad
Senior Advisor Per T. Roterud

Laboratory personnel
Senior Engineer Ingunn Tanem
Engineer Camilla Otterlei
Engineer Merete Wiig

KinCat members spring 2010

1st row: Navaneethan Muthuswany, Hassan Dar, Li He, Xuyen Kim Phan, Estelle Vanhaecke, Sara Boullosa Eiras, Fatemeh Hayer, Oana Mihai, Tayyaba Noor, Saima Sultana Kazi, Charita Udani, Nicla Vicinanza, Hilde J. Venvik.
2nd row: Karin W. Dragsten, Ingvild Tronstad, Paul Radstake, Fan Huang, Daham Gunawardana, Shreyas Rane, Anna Lind, Nina Hammer, Camilla Otterlei, Merete Wiig, De Chen, Ingvar Kvande, Rune Lødeng, Tiejun Zhao, Hongmin Wang.
3rd row: Alexey Voronov, Asmira Delic, Ilya Gorelkin, Svatopluk Chytil, Miroslav Surma, Torbjørn Gjervan, Magnus Rønning, Anders Holmen, Edd A. Blekkan, Hamidreza Bakhtiary, Eleni Patanou, Nikolas Tsakoumis, Rune Myrstad, Håkon Bergem, Asbjørn Lindvåg, Espen Wangen.

Not present: Jia Yang, Hilde Meland, Ingunn Tanem, Hoang Ahn Dam, Bjørn Christian Enger, Jun Zhu, Ingeborg-Helene Svenum.

Research Areas

- **Conversion of Natural Gas**
  - Synthesis Gas and Hydrogen Production
  - Fischer-Tropsch Synthesis
  - Dehydrogenation of Ethane and Propane
  - Solid acceptors for CO_2-capture
  - Production of Methanol and Dimethyl ether (DME)

- **Upgrading of Oil Fractions**
  - Hydrotreating
  - Catalytic Reforming/Isomerization
  - Heavy Oil Characterization and Upgrading

- **Environmental Catalysis**
  - Sulfur Reduction by Hydrotreating
  - Free Radical Chain Reactions
  - Partial Oxidation of Methane and NGL compounds
  - Preferential oxidation of CO
  - Wastewater treatment

- **Fundamental Studies of Heterogeneous Catalysis**
  - Surface Science
  - Preparation of Catalytic Materials (supported metals and metal oxides, zeolites, supports, nanoparticles)
  - Kinetics (steady-state and transient kinetics, SSITKA)
  - Adsorption and Diffusion in Porous Media
  - Catalyst Deactivation (sintering, coke formation)
  - Characterization of Heterogeneous Catalysts
  - Reactor, Kinetic and First Principles (DFT) Modelling

- **Microstructured reactors and Membrane reactors**

- **Production and Application of Carbon Nanofibers**

- **Photocatalysis**
  - Water splitting
  - Photoreforming

- **Biofuels**
  - Biomass gasification reforming and water-gas shift

- Bioethanol steam reforming
- Hydrogenation of bio-oils to biofuel diesel

Main Laboratory Equipment

- **Reaction Laboratories**

- Small pilot plants for catalytic reforming/isomerization and hydrotreating/ hydrocracking
- Several set-ups for high pressure reactions as well as for reactions at atmospheric pressure
- Conventional microbalance reactors
- Oscillating microbalance reactors (TEOM)
- Dedicated laboratory for studying microreactor technology
- Membrane reactor laboratory
- Several CSTR reactors: Berty and Caldwell reactors
- Transient kinetics (Steady-State Isotopic Transient Kinetic Analysis)
- Multireactor system for CNF synthesis

- **Catalyst Preparation Laboratory**

- **Catalyst Characterization**

- Surface area (BET), porosity and pore size distributions
- Chemisorption
- TP methods (temperature programmed methods such as TPR, TPO, TPD)
- TGA and DSC
- Raman and IR spectroscopy (in co-operation with Ugelstad Laboratory)
- Acidity determination by TPD
- UV-VIS (Avaspec 7048 UB)
- Scanning tunneling microscopy (STM) – in co-operation with Dept. of Physics.
- The following methods are available at NTNU: EM (electron microscopy), XPS (X-ray photoelectron spectroscopy), AES (auger electron spectroscopy), NMR, AFM (atomic force microscopy) and XRD (X-ray diffraction).
- Synchrotron radiation EXAFS and XRD are frequently used through ESRF and other facilities.

Activities in 2009

- The main research laboratories of the Catalysis Group are being completely renovated (October 2009 – May 2010).
- The Group is established as a Gemini centre (twin research centre).
- The Group has been evaluated together with all Chemistry groups in Norway (Hawkins Report 2009). Catalysis has a strong position in Norway and the same holds for the entire Department of Chemical Engineering.
- Hilde Venvik was spending a sabbatical leave during 2008/2009 at the University of Wisconsin-Madison, USA.
- De Chen is spending a sabbatical leave during 2009/2010 at the University of California at Berkeley, USA.
- Two group members – Edd A. Blekkan and Kjell Moljord – received the Faculty award for excellence in teaching.
- The Group participates in inGAP(Innovative Natural Gas Processes and Products) – a Centre for Research–based Innovation with participation from the University of Oslo, SINTEF, Norwegian University of Science and Technology, Statoil/Hydro, Ineos, Borealis and Halldor Topsøe AS.
- Hilde Venvik is appointed as the director for the Gas Tecnology Centre NTNU-SINTEF.
- The Norwegian Catalysis Symposium was arranged by the Catalysis group in Trondheim. The programme is enclosed. Several seminars were arranged with international participants. The programs are enclosed.
- Strategic support from NTNU (from the main administration as well as from the faculty) consisting of PhD scholarships and financial support.
- The Group participates in two European projects, one devoted to advanced cleaning for production of synthesis gas and the other to waste water treatment.
- Members of the Group participate in the Eurokin network and in large national research programs such as GASSMAKS, NANOMAT, PETROMAKS, RENERGI, KOSK.

Ph.D Candidate and Postdoctoral Projects

Experimental and modeling study of methanol synthesis in an integrated Micro Packed Bed Reactor- Heat Exchanger (IMPBRHE)

Ph.D. candidate: Hamidreza Bakhtiary,
Supervisors: Prof. Anders Holmen, Assoc. Prof. Hilde Venvik, Rune Myrstad, Sintef Materials and Chemistry

Microstructured reactors, where chemical reactions take place in channel or slit-like arrangements in the sub-millimeter range, have emerged since the early 1990ies. They have been prospected to significantly increase the efficiency relative to existing process technology because of their special characteristics in terms of mass and heat transfer. Off-shore conversions of natural gas to synthesis gas, followed by the Fischer-Tropsch synthesis or production of methanol are typical examples here.

As a work-package under a large research project of "enabling production of remote gas", the present study aims identification and evaluation of new robust and compact synthesis concepts that enables offshore GTL technology with main focus on methanol.

In this project, different key characteristics of a laboratory scale tubular Fixed Bed Reactor (FBR) with three different dilution ratios and a multichannel Integrated Micro Packed Bed Reactor-Heat Exchanger (IMPBRHE) were investigated from reaction engineering perspective in order to perform a comprehensive reactor performance comparison. The performance of each reactor was splitted into essential contributing parameters such as thermal stability and heat transfer capability, pressure drop, blank activity of wall materials and residence time distribution. The IMPBRHE The activity of CuO/ZnO/support commercial catalyst for the methanol synthesis from syngas was measured in the two reactors type. The results show that activity level in FBR is significantly affected by measured temperature gradients along the axis which could be an indication of heat transfer limitations in the undiluted FBR. The IMPBRHE however outperforms the undiluted FBR and shows a comparable conversion as compared with diluted FBRs. It was also found out that pressure drop is not a main concern in application of micro packed bed for methanol synthesis.

A 2D pseudo-homogenous model for IMPBRHE has been developed using COMSOL Multiphysics. The model applies mass and energy equations coupled with reaction kinetics in a single channel filled with small catalyst particles. The simulation results were validated by experimental data showing isothermal operation of the channels. The predicted CO conversion level by the model is in a good agreement with experimental data within an acceptable accuracy.

Publications:

1. H. Bakhtiary D., F. Hayer, X. Kim Phan, R. Myrstad, H. J. Venvik, P. Pfeifer, A. Holmen, *Experimental Study of Methanol Synthesis in a Microchannel Reactor*, Oral Presentation at 21st North American Catalysis Society meeting, San Francisco, USA, June 2009

2. H. Bakhtiary D., F. Hayer, X. Kim Phan, R. Myrstad, H. J. Venvik, P. Pfeifer, A. Holmen*, Intensification of methanol synthesis in a short contact time microstructured reactor*, Norwegian Symposium on Catalysis, Trondheim, Nov. 2009

Financial Support: StatoilHydro, UOP, Bayerngas Norge, Aker Solutions, DNV and the Research Council of Norway (168223/S30)

Development of catalytic systems for production of synthesis gas/hydrogen in membrane reactors

PhD.candidate: Hoang Anh Dam
Supervisors: Prof. De Chen, Prof. Anders Holmen

Steam reforming of CH_4 is the most common process for hydrogen production in industrial scale. The most widely used catalysts for catalytic reforming of methane are Ni supported catalysts, due to their low cost and good catalytic activity. However, the carbon formation on nickel surfaces is a serious obstacle. It is known that catalysts based on noble metals are less sensitive to coking compared to nickel-based catalysts, unfortunately, the high cost and limited availability of noble metals constrain their application in industrial practice. A combination of Ni and noble metals to form bimetallic surface alloy catalyst, using surface redox method which the surface composition is precisely controlled, is a very promising approach to solve above problems.

The bimetallic Ni(M)/HT catalysts supported on hydrotalcite-like material (HT) were prepared with various M/Ni ratios on the surfaces of Ni nanoparticles (M: Ag, Pt, Pd, Ru, Re, or Rh). Surface alloying of M with Ni influenced both the activity and the activation energy in the CH_4 steam reforming reaction, and these changes were the function of the surface M/Ni ratio. The addition of the second noble metal M significantly suppressed the carbon formation.

Kinetic studies of the carbon formation by methane decomposition on these catalysts were performed in a fixed bed reactor. The temperature ranged from 500 to 600°C. A gas mixture of CH_4 (50 ml/min) and Ar (30 ml/min) was used. The carbon formation rates of bimetallic Ni(M) /HT catalysts are extremely low, whereas the pure Ni catalyst rapidly forms carbon. Thus, the Ni-M catalysts exhibiting the surface alloy are more resistant toward carbon formation than the pure Ni catalyst.

Effects of the surface alloy of M with Ni catalysts were further investigated in the CH_4 partial oxidation reaction (POM) in a fixed bed reactor. It was found that the M addition to Ni catalyst influenced the temperature start of reaction, H_2 selectivity and CO selectivity.

Financial support:
The Research Council of Norway and Norwegian Industry

Reactor Design and Simulation for Oxidative Dehydrogenation of Ethane to Ethylene

PhD Student: Hassan Jamil Dar
Supervisor: Prof. De Chen
Co-Supervisor: Prof. Hugo A. Jakobsen

Ethylene is produced in the petrochemical industry by steam cracking. In this process, gaseous or light liquid hydrocarbons are heated to 750–950 °C.

By introducing oxygen to an ethane feed, ethylene can be produced via oxidative dehydrogenation of ethane (ODE). Oxidative dehydrogenation of ethane holds the promise of being an interesting alternative to steam cracking for ethylene production. Oxidative dehydrogenation of ethane converts ethane directly into ethylene and removes the thermodynamic limitations seen in steam cracking. It will also reduce the reactor volume.

The goal of the project is to optimize the reactor design for the maximum yield of ethylene. The following objectives will be helpful in achieving the goal of the project:

- Get a reliable kinetic model to describe the chemistry of oxidative dehydrogenation of ethane in the gas phase
- Develop proper model to describe the tublar reactor
- Design the reactor and optimize the temperature profile in the reactor to get better yield

Financial support:
The project is funded by The Research Council of Norway through the inGAP programme.

Hydrogen production by photocatalytic water splitting

Ph.D. candidate: Asmira Delic
Supervisor: Prof. Magnus Rønning

Photocatalytic water splitting using sunlight is an environmentally clean alternative to hydrogen production from fossil fuels. In photocatalysis photochemical reactions take place at a solid surface, usually a semiconductor. Upon illumination the semiconductor becomes catalytically active when photoelectrons and photo-holes are generated. In water splitting the holes oxidize water to O_2 and protons. The electrons reduce protons to H_2. The most appropriate semiconductor for photocatalytic reactions is considered to be TiO_2. Currently there are two major challenges regarding the use of TiO_2 for photocatalytic water splitting. The first problem is deactivation through recombination of the photogenerated electron-hole pairs. The second problem is that the material is active upon UV radiation and not visible light, which is the main part of the solar spectrum. The goal of this project is to address these problems though modifying the TiO_2 catalyst.

A promising approach for suppressing the recombination of electron-hole pairs is to couple TiO_2 with carbon-based materials. The synergetic effects depend on the type of carbon material as well as the synthesis route of the TiO_2–carbon composites. Photo-response in the visible light region can be achieved through doping of TiO_2 with certain anionic species such as nitrogen, carbon and sulphur.

This project explores the structure and function of composites with different dopants, different TiO_2:CNT ratios, different types of carbon nanotubes (CNT) and with TiO_2 located inside and outside the carbon nanotubes. The CNT are prepared by CVD on porous carbon support, with subsequent decoration of the tubes by TiO_2. The structure and morphology of the catalysts are investigated by characterization techniques such as TEM, SEM, XRD, BET, TGA and Raman spectroscopy. Assemblies of TiO_2-CNT/Nafion/Pt are used to test the photocatalytic activity. In a photoelectrochemical reactor H_2 and O_2 are produced in separate chambers, resembling a reversed fuel cell. The catalytic activity is evaluated by measuring the rate of H_2 and O_2 evolution.

Financial support:
Strategic funding, NTNU.

Comparative study of selected catalysts for catalytic partial oxidation of natural gas.

PhD candidate: Sara Boullosa Eiras
Supervisors: Prof. Anders Holmen, Prof. De Chen

Conversion of methane can be carried out in two ways, either directly or via synthesis gas. Most commercial processes for production of chemicals, fuels or hydrogen follow the syngas route. Steam reforming is the main process for converting methane to hydrogen, in fact more than 90 % of the global hydrogen is produced by steam reforming. Oxidative concepts like autothermal reforming and catalytic partial oxidation are also attractive processes for production of synthesis gas. Autothermal reforming is already a commercial process, whereas catalytic partial oxidation has not yet been commercialized. Catalytic partial oxidation (CPO) of methane could have several advantages compared to other technologies such as high space velocities (compact reactors), fast responses in dynamic operations and a molar ratio H_2 / CO of about 2. In addition, the partial oxidation $CH_4 + 1/2O_2 \rightarrow CO + 2H_2$ is only weakly exothermic.

This project deals with catalytic partial oxidation of natural gas to synthesis gas. High temperature resistant materials are required for applications like CPO where the temperature in the catalytic bed can be over 1273 K. To obtain catalysts with high activity and stability, it is fundamental to avoid the sintering to maintain the dispersion of the active phase. Alumina is widely used as a catalyst support because of its high surface area and thermal stability. However, the specific surface area of alumina deteriorates remarkably above 1273 K owing to sintering and phase transition to α-alumina. For the suppression of the phase transformation additives such as Ce, Zr, La, or Ba can be added. In this project the effect of the addition of ZrxCe1-xO2 to the alumina support is studied.

The project is part of a large research effort in the catalysis group dealing with the conversion of methane.

Publications and presentations:

1. S. Boullosa-Eiras, T. Zhao, Y. Yu, D. Chen, A. Holmen. *Supported Rh on ZrO_2-Al_2O_3 nanocomposite catalyst for catalytic partial oxidation of methane to syngas.* Poster presentation. 6th World Congress on Oxidation Catalysis, 5-10 July 2009, Lille, France.
2. S. Boullosa Eiras, T. Zhao, Y. Yu, D. Chen, A. Holmen. *Alumina-based nanocomposite supported Rh catalysts: an effective and highly stable catalyst for partial oxidation of methane to syngas.* Poster presentation. EuropaCat2009, 30 August – 4 September 2009, Salamanca, Spain.
3. T. Zhao, S. Boullosa-Eiras, Y. Yingda, Y. Xiaofeng, S. Raaen, M. Ronning, D. Chen, A. Holmen. *Synthesis and catalytic performance of high-temperature stable nanocomposites by a versatile nanoparticle-*

mediated Pechini method. Oral presentation. EuropaCat2009, 30 August – 4 September 2009, Salamanca, Spain.

4. Holmen, B. C. Enger, R. Lødeng, S. Boullosa-Eiras and D. Chen. *Partial oxidation of methane.* Oral presentation. AIChE Annual Meeting 2009. 8-13 November 2009, Nashville, USA.
5. S. Boullosa-Eiras, T. Zhao, E. Vanhaecke, Y. Yu, D. Chen, A. Holmen. *Ce-Zr-Al mixed oxide nanocomposites supported Rh: a promising catalyst for partial oxidation of methane to syngas*. Poster presentation. Norwegian catalysis symposium 2009, 30 November – 1 December 2009, Trondheim, Norway.
6. S. Boullosa-Eiras, E. Vanhaecke, T. Zhao, D. Chen, A. Holmen. *Raman and X-ray investigations of the phase transformation of ZrO2-Al2O3 and CeO2-Al2O3 nanocomposites.* Accepted for Catalysis Today.
7. S. Boullosa-Eiras, T. Zhao, E. Vanhaecke, Y. Yu, D. Chen, A. Holmen *On the thermal stability and catalytic performance of Rh/CexZr1-xO$_2$/Al$_2$O$_3$ nanocomposites prepared through a modified pechini sol-gel method*. In preparation.

Financial Support:
The project is funded by The Research Council of Norway (NFR), and Statoil.

New concepts in the catalytic dehydrogenation of propane

Ph.D. candidate: Ilya V. Gorelkin
Supervisor: Prof. Edd A. Blekkan

The production of light alkenes (C_2-C_4) is a central part of the petrochemical industry. Due to a higher growth in the demand for propene compared to other alkenes, the selective production of propene via catalytic dehydrogenation of propane is interesting. Here we propose to work on fundamental and applied issues in propane dehydrogenation, mainly the development of a new concept in process heating, based on the *in situ* catalytic combustion of hydrogen, at conventional processing conditions for propane dehydrogenation, i.e. around 600 °C. The subject of study are reactions between hydrogen and oxygen on supported noble metal catalysts (platinum, iridium, and bimetallic systems involving these and other metals) in the presence of hydrocarbons (propane, propene) and microkinetic modelling of such reactions.

Financial Support:
The project is funded by the Research Council of Norway under the GASSMAKS research program.

New approach to metal dusting corrosion

Ph.D. candidate: Panditha Vidana Daham Sanjaya Gunawardana
Supervisors: Assoc. Prof. Hilde Venvik and Prof. De Chen

Metal dusting is a catastrophic corrosive degradation phenomenon on metals and alloys that proceeds by a gradual breakdown of the material into fine particles. It constitutes a problem in the chemical and petrochemical industries, where metals and alloys extensively exposed to carbon-supersaturated gaseous environment ($a_C > 1$) with low partial pressures of oxygen or steam in a critical temperature range of 300–900 oC. Metal dusting carries significant cost which is associated with application of certain precautionary measures and ultimate replacement of certain process unit and equipment. In this study, we are focusing on understanding the metal dusting mechanism and finding out the controlling variables of metal dusting in the point of view of methanol synthesis technology. An overall objective will be to develop predictive tools for the metal dusting induction.

The project has a multidisciplinary approach that includes experimental and theoretical studies of metal dusting combined with novel surface and bulk characterization. Model alloy samples are tested under controlled conditions, and assessment of mass change under relevant reaction conditions can be applied to obtain the rate of metal dusting. Available techniques for investigation of the surface and bulk morphology and composition include TEM, SEM, AFM, STM, XRD, EDXS, AES and XPS, as well as IR and Raman spectroscopic techniques. Modelling will be applied to understand better the initial steps leading to the formation of elemental carbon.

Financial support:
The project is funded by The Research Council of Norway through the inGAP programme.

Compact Production of Di-Methyl-Ether (DME)

PhD-candidate: Fatemeh Hayer
Supervisors: Assoc. Prof. Hilde J. Venvik, Prof. Anders Holmen

Dimethyl ether (DME) is the simplest ether, and it has emerged as a clean substitute for auto diesel fuel with reduced exhausted emissions. .It could be processed under LPG technology to use for heating and home cooking. It has also been introduced as an aerosol propellant in spray cans.

The objective of this project is to produce DME directly from syngas via methanol synthesis and methanol dehydration in the same reactor. The process is highly exothermic and required a catalyst with syngas hydrogenation and methanol dehydration sites. High DME production and high one pass CO conversion are objected to many issues; syngas composition, pressure,

temperature, residence time and catalyst system. A heat exchange, microchannel reactor with high area to volume ratio and laboratory fixed bed reactor are applied to study of DME synthesis. The reactors are packed with a physical catalyst mixture (weight ratio 1:1) prepared by methanol synthesis catalyst CuO-ZnO-Al_2O_3 and methanol dehydration catalyst either HZSM-5 or γ-Al_2O_3. HZSM-5 as a dehydration catalyst was superior to γ-Al_2O_3 with respect to productivity, selectivity and stability. However, in the point of reactor loading, γ-Al_2O_3 introduces a more convenient procedure. The experiment to achieve an optimum composition of hybrid catalyst is going on. . The experiments reveals that a H_2:CO ratio of 1~2 is optimum for high productivity. However, regarding achieving high CO conversion at 50 bar and 250°C, H_2:CO close to 2 could be optimum if the objective is a maximized single pass CO conversion.

Financial support:
The project is funded by the Research Council of Norway under the GASSMAKS research program.

A direct production approach from biomass to very pure H_2

Ph.D. candidate: Li He
Supervisor: Prof. De Chen

An attempt has been made to develop a flexible system to produce very pure H_2 with high efficiency from renewable bio-based recourses. First, such model compounds as ethanol, glycerol, sorbitol and glucose, have been tested for H_2 production via sorption enhanced steam reforming (SESR) over Co-Ni/hydrotalcite-like (HTls) derived catalyst and CaO-based CO_2 acceptor. The experimental results show that all of feedstocks, even heavy feedstocks, were able to offer high H_2 purity (97.3~99.1%) and yield at low steam to carbon (S/C = 1.3~6) ratio in comparison to the corresponding steam reforming process. In addition, the studied system also presents encouraging potential for improvement of energy efficiency. Chemical looping combustion (CLC) was coupled to the cyclic multi-step SESR process to assist the acceptor regeneration by using multifunctional Pd/Co-Ni/HTls catalyst. With coupling of CLC to SESR, H_2 concentration in the gas effluent of the SESR reactions was still higher than 95 mol% on a dry basis. The assembled CLC-SESR process has inherent high efficiency in H_2 production.

Publications:

1. Li He and De Chen: *Novel Materials in H_2 Production by CO_2 Sorption Enhanced Steam Reforming*, , book chapter, Sorption enhanced reaction (SER) concepts for hydrogen production, Editor: Dr. Shivaji Sircar and Dr. Ki Bong Lee, Research Signpost/Transworld Research Network.

2. Li He, Helene Berntsen and De Chen: *Approaching Efficient H_2 production: Sorption Enhanced Steam Reforming of Ethanol*, Journal of Physical Chemistry: A. (2009) DOI: 10.1021/jp906146y.
3. Li He, Jacobo Manuel Salamanca Parra, Edd Anders Blekkan and De Chen: *Towards efficient hydrogen production from glycerol by sorption enhanced steam reforming*, submitted to Energy & Environmental Science
4. Li He, De Chen: *Generating High-Purity Hydrogen From Biomass in One Reactor via Sorption Enhanced Steam Reforming*, submitted.

Presentations:

1. Li He, De Chen, Submitted abstract, *Coupling CO_2 Capture in Catalytic reactions for the Conversion of Biomass to H_2.* The ninth edition of the Novel Gas Conversion Symposium (NGCS 9), May 30th – June 3rd, 2010, Lyon, France.
2. Li He, Tiejun Zhao, Kazi Saima Sultana, Magus Rønning, De Chen, keynote lecture, *Progress in Carbonate Looping Process: Material and Applications*. 239th National Meeting of the American Chemical Society, March 21-25, 2010, San Francisco, California, USA.
3. Li He, De Chen, submitted abstract, *Highly Efficient Hydrogen production from Biomass.* 239th National Meeting of the American Chemical Society, March 21-25, 2010, San Francisco, California, USA.
4. Li He, Morten Beinset, Helene Berntsen, De Chen, Oral, *Mulifuctional Composites for H2 production via Sorption Enhanced Steam Reforming,* 2009 – EuropaCat IX Congress, August 30 – September 4,2009, Spain.

Financial support:
The project is funded by The Research Council of Norway.

In-situ Polymerization of Conducting Polymers on CNT/CNF

Ph.D. candidate: Fan Huang
Supervisor: Prof. De Chen

This project focuses on the examination of the in-situ polymerization of different conducting polymers on carbon nanostructures and the determination of the properties, such as electrochemical behavior, thermal stability, of the composites. The application of these composites is wide and interesting, for example, the usage of the conducting polymer/CNT composite in supercapacitor.

The electrical-chemical properties of chemically in-situ polymerizaed PANI on aligned CNT were examined. From the cyclic voltammetry test, it was found the specific capacitance of the composite is 452 F/g, power density 5.17 KW/Kg and the energy density 57.4 Wh/Kg. Following the previous chemical in situ polymerization of PANI on both non-aligned and aligned CNT, PANI was also in-situ polymerized on aligned CNT electro-chemically. It was found the

polymer coating was more homogeneous than that synthesized in the chemical way. And one important advantage is that the amount of PANI can be easily controlled by changing the power input duration from the potentiostat.

In-situ polymerization of PANI on fishbone and platelet carbon nanofibers, nitrogen doped carbon nanotubes. The chemical structure of the polyaniline on these carbon nanostructures was the same as PANI/non-aligned CNT composites from the Raman results, indicating that the carbon nanostructures don't have much influence on the chemical structure of PANI.

Publications and presentations in 2009:

1. Fan Huang, Estelle Vanhaecke, De Chen, *In-situ polymerization and characterizations of polyaniline on MWCNT powders and aligned MWCNT films*, 2009, Catalysis Today—Accepted
2. Fan Huang, Estelle Vanhaecke, De Chen, *In-situ polymerization and property of PANI /CNT composite*, Nanolab seminar, 2009.
3. Estelle Vanhaecke, Fan Huang, De Chen, Magnus Rønning, *Carbonnanotubes Synthesis on Foils*, Vista StatoilHydro, 2009.

Financial support:
The Research Council of Norway (NFR)

Hydrogen Production by Sorbent Enhanced Reforming (SER)

Ph.D. candidate: Kazi Saima Sultana
Supervisor: Prof. De Chen

Sorption-enhanced steam reforming of methane is a process, in which steam reforming reaction is carried out in the presence of CO_2 sorbent. In a Sorption-enhanced reactor, CO_2 is captured by a sorbent and the reverse reaction cannot take place. So the equilibrium is shifted to the product (hydrogen) side. This makes it possible to run the steam reforming reaction at much lower temperature (400 - 500°C instead of 800 - 900°C).

The project focused on developing of new calcium based CO_2 acceptors. The new sorbents are prepared by spray drying technique. The prepared sorbents are studied by different techniques including scanning electron microscope (SEM), transmission electron microscope (TEM), X-ray diffraction (XRD), XPS, TGA to find information about the morphology, stability and capacity of the sorbents.

Among the prepared sorbents CaCe (10:1), CaCeZr (10:1:1) and CaZr (8:1) mixed oxides have shown a very promising property for CO_2 capture. These oxides have stable capacity 0.53, 0.46 and 0.45 (g of CO_2/ g of sorbent) respectively for 20 cycles. Sorption capacity of CaAl (8:1) and CaAlMg (10:1:1) mixed oxide sorbents are lower 0.25 and 0.30 (g of CO_2/g of sorbent) compared to other mixed oxides after 20 cycles. Experimental performance of hydrogen

production by sorption enhanced methane reforming (SESMR) is performed in a fixed bed reactor by installing Ni-based catalyst, Ni-HT (~40 wt % NiO) and mixed oxide sorbent. In practical application, the Ca-based sorbents are repeatedly used; that is, the sorbents must be regenerated in cycles after the carbonation reaction. Therefore, the repeated carbonation/calcination cycles of sorbents are studied for SESMR. It has been found that prepared Ca –based sorbents can adsorb sufficient CO_2 to enhance the CH_4 conversion and almost 95%+ hydrogen are obtained. Kinetic study the sorbents will also be studied under different partial pressures of CO_2, steam and at different temperatures.

Presentations in 2009:

1. Kazi Saima Sultana, Tiejun Zhao, Siri Albertsen Fagerbekk, Li He and De Chen: *Calcium based sorbents for CO_2 capture in sorption enhanced steam methane reforming*.Lecture: 10th International Conference on CO_2 Utilization (ICCDU-X), Tianjin, May 17-21, 2009.
2. Tayyaba Noor, Kazi Saima Sultana, and De Chen: *Development and Testing of Mixed Oxides Nanoparticles For Carbon Dioxide Capture in Sorption Enhanced Reactions.* Poster: InGAP NANOCAT Summer School Trondheim, Norway, June 21-26, 2009.
3. Kazi Saima Sultana, Estelle Vanhaecke, Tiejun Zhao, Magnus Rønning and De Chen: Sol-Gel Derived Zirconia *Coated Calcium Oxide Nanoparticles for CO_2Capture*. Lecture: Norwegian Catalysis Symposium, Trondheim, Norway, November 30-December 1, 2009.

Financial support:
The project is funded by The Research Council of Norway.

Properties and application of 1-5 µm Pd/Ag23wt.% membranes for hydrogen separation

Ph.D. candidate: Astrid Lervik Mejdell
Supervisors: Ass. Prof. Hilde J. Venvik, Dr. Scient. Rune Bredesen, SINTEF

Thin (1-5 µm) Pd/Ag23wt.% films were produced by magnetron sputtering and subsequently removed from the sputtering substrate and applied to either a flat configuration with the gas flowing perpendicular to the surface or a microchannel configuration with the gas flowing along the membrane in parallel channels. The membrane hydrogen transport was studied under different conditions to investigate factors such as thickness dependent behaviour, concentration polarisation, and competitive adsorption by other gas species as well as the effect of membrane heat treatment in air.

Under H_2:N_2 mixtures, large concentration polarisation (gas phase transport) effects existed in the flat configuration, but had minor impact in the

microchannel configuration. The membranes could withstand high differential pressures (>470 kPa) when supported by the microchannel structure, conveniently enabling hydrogen separation without the use of a permeate side sweep gas. Permeance values were determined under pure hydrogen feed and no sweep gas after initial stabilization. A correlation between hydrogen flux and membrane thickness was obtained, but permeability variations within sputtering batches as well as between batches were observed that indicate bulk diffusion not being the sole rate-limiting step. The application of a thermal treatment in air procedure resulted in significantly improved permeance, particularly for the thinnest membranes. The permeability values became more uniform ($\sim 2.1 \cdot 10^{-8}$ $mol \cdot m \cdot m^{-2} \cdot s^{-1} \cdot Pa^{-0.5}$) and bulk diffusion was rate limiting. Atomic force microscopy investigations showed a correlation between increased permeation and increased surface area, roughness and grain size.

CO had strong inhibiting effects on hydrogen permeation, however decreasing upon increasing the temperature from 275 to 350 °C. CO_2 was found to have minor effect at 350 °C, while 10 mol% CO_2 at 300 °C led to a steady decrease over time. Competitive adsorption is the main mechanism for CO inhibition, while the inhibiting effect of CO_2 seems to be caused by slow formation of strongly adsorbed species. The thermal treatment in air led to a significant reduction in the CO inhibition. An approach combining a Sieverts-Langmuir and microkinetic modelling (through transition state and unity bond index-quadratic exponential potential theories) indicates that the change in CO inhibition effect can at least partly be explained by changes in the CO and H_2 heats of adsorption. No permeation decrease under CO_2 exposure was observed after heat treatment in air.

The research is performed in collaboration with SINTEF Materials and Chemistry, Energy Conversion and Materials Department. Astrid L. Mejdell defended her PhD thesis on 2009-05-08and is now employed by Statoil ASA.

Publications and presentations:

1. A.L. Mejdell, M. Jøndahl, T.A. Peters, R. Bredesen, H.J. Venvik: *Experimental investigation of a microchannel membrane configuration with a 1.4 μm Pd/Ag23% membrane – effects of flow and pressure.* Journal of Membrane Science 327 (2009) 6.
2. A.L. Mejdell, T.A. Peters, M. Stange, H.J. Venvik, R. Bredesen: *Performance and application of thin Pd-alloy hydrogen separation membranes in different configurations*. J. Taiwan Inst. Chem. Eng. 40 (2009) 253.
3. A.L. Mejdell, M. Jøndahl, T.A. Peters, R. Bredesen, H.J. Venvik: *Effects of CO and CO2 on hydrogen permeation through a ~3 μm Pd/Ag 23wt.% membrane employed in a microchannel membrane reactor configuration*. Separation and Purification Technology 68 (2009) 178.

4. A.L. Mejdell, D. Chen, T.A. Peters, R. Bredesen, H.J. Venvik: *The effect of heat treatment in air on CO inhibition of a ~3 μm Pd/Ag 23wt.% membrane*. Journal of Membrane Science 350 (2010) 371.
5. A. Ramachandran, W.M. Tucho, A.L. Mejdell, M. Stange, H.J. Venvik, J. Walmsley, R. Holmestad, R. Bredesen, A. Borg: *Surface characterization of Pd/Ag23wt% membranes after different thermal treatments*. Submitted.
6. A.L. Mejdell, T.A. Peters, R. Bredesen, D. Chen, H.J. Venvik: *1.5-3 μm Pd/23wt.%Ag membranes applied in a microchannel membrane configuration - effects of flow, pressure and competitive adsorption of CO and CO_2.* ICOSCAR-3, 3rd International Conference on STRUCTURED CATALYSTS AND REACTORS; 2009-09-27 - 2009-09-30

Financial support:
The project is funded by the Research Council of Norway (RENERGI programme) through the NTNU-SINTEF Gas Technology Center, with supplementary funding from the KOSK programme (Contract No. 135938/431) and the NANOMAT programme (Contract No.: 158516/S10) and Statoil ASA.

Partial oxidation of methane. Studies on mechanism and kinetics

Ph.D. candidate: Oana Mihai
Supervisors: Prof. Anders Holmen and Prof. De Chen

The purpose of the research project is to understand the kinetics and mechanism of methane partial oxidation process with no presence of gas phase oxygen. The reaction is based on methane feeding by using lattice oxygen of perovskites oxides type $LaFeO_3$ as oxygen source. The work involves the studies regarding the reaction mechanism and the optimization of catalyst composition in order to obtain maximum yield of synthesis gas.
Partial oxidation is weakly exothermic reaction meaning that less heat is needed:

$$CH_4 + ½\ O_2 = CO + H_2 \qquad \Delta H_{298K} = -36\ kJ/mol$$

Both the preparation and characterization of catalyts are important parts of this work. The experiments were carried out using a fixed bed quartz micro reactor with the catalyst sample fixed on a sinter and performed at high temperatures in the range of 780ºC to 900ºC, atmospheric pressure and various flow rates. The process is simulated by a redox cycle, switching between oxygen flow diluted in argon followed by methane flow diluted in argon. In order to avoid the mixing of methane and oxygen in gas phase, the reactor system was flushed with argon between the oxidation and reduction steps.

The Fe perovskites are suitable catalysts for partial oxidation process due to their ability to utilize a large part of its lattice oxygen during reaction, a good thermal stability. The properties of surface and bulk oxygen are also important. Reactive surface oxygen will give total CH_4 combustion to CO_2 and H_2O while the bulk oxygen can react with CH_4 to give selective oxidation products as CO

and H_2. An important part of this work will be to determine the surface reaction mechanisms.

Presentations in 2009:

1. O. Mihai, D. Chen, A.Holmen: *Comparative study regarding preparation methods of perovskite-type oxides $LaFeO_3$ catalysts for methane partial oxidation.* Poster. inGAP-NANOCAT Summer School, Trondheim, Norway, June 21-26, 2009.
2. O. Mihai, D. Chen, A.Holmen: *Synthesis of perovskites using carbon nanotubes as templates as their applications in methane partial oxidation.* Poster. Norwegian Symposium on Catalysis, Trondheim, Norway, November 30, 2009.

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The project is funded by The Research Council of Norway through the KOSK programme

Synthesis and characterization of bimetallic nanoparticles supported on Carbon materials for fuel cell applications

Ph.D. cadidate: Navaneethan Muthuswamy
Supervisors: Prof. De. Chen and Prof. Magnus Rønning

The main objective of this assignment is developing high efficient electro catalyst for Fuel Cell devices with well dispersed bi-metallic loading in the form of nanoparticles over carbon materials and to investigate the role of second metal to minimize the rate of deactivation (due to sintering and blocking of active sites by CO) during electrode reaction.

In recent years, the investigation have been focused on the application of nanostructured materials for developing high efficient polymer electrolyte membrane fuel cell (PEMFC) in order to overcome the fast depletion of fossil fuels and to meet the challenge of global warming. But in fuel cell application, Pt is regarded as the best catalyst for electrochemical reactions (both anode and cathode) such as hydrogen oxidation reaction (HOR) and oxygen reduction reaction (ORR). Its high costs, limited supplies and low stability (due to poisoning effect by CO) are the major problem in commercialization of fuel cells. So recently synthesis of core-shell system with thin layer of catalytically active Pt metals on the other metal cores has been much focused. By achiving this system not only reduces the Pt loading but also enhances the stability of the catalyst via the so-called ligand effects, where the core metal modifies the electronic structure of the Pt by donating electron density. Thus, the Pt-CO bond strength weakens and therby allowing CO to be more easily oxidized by OH molecules adsorbed at the neighbouring Pt surface. But still the meachanism is under debate.

Preparation of an active catalyst with well dispersed bimetallic (core-shell) nanoparticles on carbon materials by polyol route can be able to increase the performance of PEMFC with decreased Pt loading.

Financial support:
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Integrated process for hydrogen production with CO_2 capture using sorption enhanced reactions

Ph.D. candidate: Tayyaba Noor
Supervisor: Prof. De Chen

Steam reforming is currently the major process for large-scale production of hydrogen. Hydrogen production from steam reforming is a process that involves multiple steps and severe operating conditions. A pre-reforming step is normally necessary to convert heavy hydrocarbons to methane and synthesis gas, in order to lower the coking potential. The methane reformer is normally operated at 800-950°C and 20-35 bar and need large amounts of energy to maintain the reaction temperature. The reformer is followed by high and low temperature water-gas shift reactors, and then carbon dioxide removal. In some cases, methanation is necessary to reduce the carbon monoxide concentration. All these steps make hydrogen production very costly. An alternative, cost-effective process for hydrogen production is therefore highly desirable.

Objectives:
1) Develop highly active and stable catalysts with high coking resistance, enabling the use of Norwegian natural gas as a feed stock for one-step, large-scale hydrogen production.

2) Explore solid CO_2 sorbents in sorption enhanced reactions for hydrogen production.

3) Test experimentally hydrogen production using sorption enhanced steam reforming of natural gas and sorption enhanced water-gas shift reaction

Hydrotalctile based Nickel catalysts have been developed using spraying drying technique. Series of catalyst have been prepared with different Ni loadings and characterized by techniques like XRD, SEM, Chemisorption and BET. A calcium, cerium, zirconium based mix oxide sorbent has also been developed. Sorbent will be installed together with catalyst in a fixed bed reactor. Both sorption enhanced steam reforming of natural gas and water gas shift reaction will be studied. The reaction conditions such as catalyst to sorbent ratio, temperature, pressure and steam to carbon ratio will be optimized in terms of hydrogen yield. Regeneration condition of the sorbents will also be studied to

lower the regeneration temperature. Stability of the materials will be tested in multi-cycle runs.

Poster Presentations:

1. Tayyaba Noor, Saima Kazi, De Chen, *Development and testing of mixed oxides nanoparticles for CO_2 capture in sorption enhanced reactions.* InGAP-Nanocat summer School, 21-26 June, 2009, Trondheim, Norway.
2. Tayyaba Noor, Anna Lind, Andres Hollmen, De Chen*, Synthesis and Characterization of Ni Hydrotalcite Catalyst for Hydrogen Production Using Co Precipitation, Spray Drying, Microemulsion Method*. Norwegian symposium on catalysis, 30 Nov-01 Dec, 2009, Trondheim, Norway.

Financial Support:
The project is funded by The Research Council of Norway through KOSK Programme.

Microcalorimetry and microkinetics of heterogeneous catalysts.

Ph.D. candidate: Eleni Patanou
Supervisor: Prof. Edd A. Blekkan
Co-supervisor: Prof. De Chen

Microkinetic modeling is very useful in the modern approach of improving and developing heterogeneous catalysts. In this project the microkinetic modelling constitutes a key tool in order to link information from theory, experimental surface science, mechanistic studies and kinetic and finally deactivation studies. The BOC theory is used as a framework where the main model input is the binding energies of the adsorbed species on the catalyst surfaces. As the amount of heat involved during the adsorption process is closely related to the adsorbate - substrate bond strength, the values of the heat of adsorption will be theoretically estimated and experimentally confirmed.

Adsorption microcalorimetry is recognized to be the most reliable method to determine the energy of the bonds between the adsorbed species and the adsorbents. Using a high sensitive Tian Calvet type calorimeter coupled to a volumetric chemisorption apparatus, the amount of the heat transferred per unit time it will be detected as a function of the amount of the probe molecule adsorbed on the catalyst. In order to preserve the surface clean from any contamination of undesirable adsorbed species the catalyst is treated in a unique cell and transferred direct from the reduction into the calorimeter to start the measurement of the adsorption heat with the chosen probe gas.

In the present work microcalorimetric results will be used to eliminate errors and to assure better fitting of the computational techniques with the experimental data for heterogeneous catalysts widely used from the group as Fischer-Tropsh catalysts.

Publications and presentations in 2009:

1. Patanou, E., Chen, D., Blekkan, A. E., *Microcalorimetry & microkinetics of heterogeneous catalysts*, Poster, InGap–Nanocat Summerschool in Heterogeneous catalysis: Nano designed catalysts: from molecules to industrial processes, 21-26 June 2009, Trondheim, Norway.
2. Patanou, E., Chen, D., Blekkan, A. E., *Microcalorimetry & microkinetics of heterogeneous catalysts*, Poster, Norwegian Catalysis Symposium 2009, November 30 - December 1 2009, Trondheim, Norway.

Financial support:
The Research Council of Norway (NFR) and industrial partners through the inGAP programme.

Preparation and Performance of a Catalyst coated Stacked Foil Microreactor for the Methanol Synthesis

Ph.D. candidate: Xuyen Kim Phan
Supervisors: Prof. Anders Holmen and Assoc. prof. Hilde J. Venvik
Project manager: Rune Myrstad

Microstructured reactors have received attention over the past two decades due to their process intensification and safety potential. This potential arises from the high surface to volume ratio that enhances mass and heat transfer, as well as from the small amount of reactants and products inside each microchannel. Using microchannels for heterogeneously catalyzed reactions introduces new challenges to catalyst loading, since filling the microchannels with catalyst powders may lead to flow maldistribution. For the option of coating the micochannel walls with catalytic materials, heat and mass transfer properties may allow coatings with even higher activity than powder filling. However, a considerable increase of surface area relative to the channel geometric area, accompanied with good adhesion on the channel walls, is demanded for the coatings. This study focuses on a microreactor configuration of stacked, catalyst coated foils for the methanol synthesis. Two catalytic coatings were prepared, Pd/CeO2 and CuO/ZnO/Al2O3, and studied under relevant conditions. A comparison to laboratory scale fixed reactor experiments has also been made. The results show that stable and active foils coatings of both Pd/CeO2 and CuO/ZnO/Al2O3 can be prepared. The activity of Pd/CeO2 coated foils is significant better than Pd/CeO2 particles prepared by deposition-precipitation method, presumably due to the different preparation techniques, while differences between two reactor types are found using the same Cu catalyst that seems to relate to temperature properties.

Publications & presentations in 2009:

1. Xuyen K. Phan, Jia Yang, Hamidreza Bakhtiary D., Rune Myrstad, Hilde Venvik, Anders Holmen. *Studies of Macroporous structured Alumina*

based Cobalt Catalysts. Poster at EuropaCat IX, Salamanca, Spain, 30th August-4th September 2009

2. Xuyen K. Phan, Hamidreza Bakhtiary D., Rune Myrstad, Janina Thormann, Peter Pfeifer, Hilde Venvik, Anders Holmen. *Experimental Study of Methanol Synthesis in a Stacked Foil Microchannel Reactor.* Poster at Norwegian Catalysis Symposim, Trondheim, Norway, 30th Nov – 1st Dec 2009
3. Xuyen K. Phan, Hamidreza Bakhtiary D., Rune Myrstad, Janina Thormann, Peter Pfeifer, Hilde Venvik, Anders Holmen. *Preparation and performance of Cu-based monoliths for methanol synthesis.* Accepted as poster presentation at Novel Gas Conversion Symposium, Lyon, France, June 2010.
4. Xuyen K. Phan, Hamidreza D. Bakhtiary, Rune Myrstad, Janina Thormann, Peter Pfeifer, Hilde J. Venvik, Anders Holmen. *Preparation and Performance of a Catalyst coated Stacked Foil Microreactor for the Methanol Synthesis.* Accepted as oral presentation at ICSRE 21, Philadelphia, USA, June 2010.
5. Xuyen K. Phan, Hamidreza D. Bakhtiary, Rune Myrstad, Janina Thormann, Peter Pfeifer, Hilde J. Venvik, Anders Holmen. *Preparation and Performance of a Catalyst coated Stacked Foil Microreactor for the Methanol Synthesis*. Manuscript in preparation.

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Dehydrogenation of NGL components at very short contact times

Ph.D. candidate: Paul B. Radstake
Supervisors: Prof. Anders Holmen, Prof. Magnus Rønning

Lower olefins such as ethene and propene are important intermediates for a large number of industrial processes. NGL (C_2-C_4 components in natural gas) is an excellent feedstock for production of lower olefins and Norway has access to large quantities of NGL. Oxidative dehydrogenation at very short contact times represents a new, exciting and promising way of converting NGL components to the corresponding olefins. It holds the promise of greatly reducing the reactor volume, as well as of autothermal operation. Another advantage is that it overcomes the thermodynamic limitations and avoids the necessity of continuous catalyst regeneration.

The purpose of the project is to characterize the oxidative dehydrogenation of NGL components at very short contact times and high temperatures. The focus of the project will be mainly on the selection of both convenient catalytic

systems and suitable characterization techniques in order to further understand the fundamentals of this type of reactions.

The experimental work will be based on wash-coated monoliths or powdered supports impregnated with either Pt-Sn or perovskites ($LaMnO_3$). Parameters to be investigated are mainly catalyst loading, atomic ratios of the different elements, type of washcoat (to be compared with the powdered supports), synthesis procedures and catalyst precursors. The characterization will be based on both physicochemical and spectroscopic techniques as well as the catalytic performance. Parameters within the catalytic testing experiments will be investigated as well. These parameters include reaction temperature, gas flow rates and gas ratios.

Financial support:
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Studies on relation between catalyst properties and selectivity in Fischer-Tropsch Synthesis

Ph.D. Candidate: Shreyas Rane
Supervisors: Prof. Anders Holmen and Dr. Øyvind Borg, Statoil.

The Fischer-Tropsch synthesis is rapidly becoming the most important technology for conversion of natural gas to liquid fuels (GTL). A key element in improved Fischer-Tropsch technology is the development of active catalysts with high wax selectivity. Supported cobalt is the preferred catalysts for the Fischer-Tropsch synthesis of long chain paraffins from natural gas due to their high activity and selectivity, low water-gas shift activity and relatively slow deactivation.

The present project deals with the study of the relation between catalyst properties and their effects on the Fischer-Tropsch synthesis. As a part of the experimental work, the supported cobalt catalysts are prepared by incipient wetness impregnation without adding any promoter. The studies involve the effect of different alumina supported catalysts with constant metal particle size of cobalt on the C_{5+} selectivity. All catalysts are characterised by standard techniques such as H_2-chemisorption, oxygen titration and TPR (Temperature Programmed Oxidation and Reduction), XRD (X-ray Diffraction), BET-surface area measurements, SEM (Scanning Electron Microscopy) and SSITKA (Steady-State Isotopic Transient Kinetic Analysis. The catalysts are tested in a fixed bed reactor at industrially relevant conditions (H_2: CO = 2, 20 bar, and 483 K).

Based on experimental results, it is concluded that the C_{5+} selectivity is dependent on the alumina phase and its pore size distribution. In order to gain theoretical understanding about variations in hydrocarbon selectivity, Raman

spectroscopy will be used. Apart from this work, the synthesis reaction was studied for carbon nanofiber/felt supported cobalt catalysts, having platelet and fishbone structure, to examine long-run stability as compared to alumina support.

Publication and presentations:

1. Shreyas P. Rane, Erik Z. Tveten, Erling Rytter, Øyvind Borg, Anders Holmen: *Performance of supported Co catalysts for Fischer-Tropsch synthesis.* Lecture, 21st NAM, San Francisco 2009.
2. Shreyas Rane, Øyvind Borg, Erling Rytter, Anders Holmen: *Effect of cobalt particle size, alumina and its porosity on hydrocarbon selectivity in Fischer-Tropsch synthesis.* Poster presentation, Norwegian Catalysis Symposium, Trondheim 2009.
3. Shreyas Rane, Øyvind Borg, Jia Yang, Erling Rytter, Anders Holmen: *Effect of alumina phases on hydrocarbon selectivity in Fischer-Tropsch synthesis*. In preparation.
4. Shreyas Rane, Øyvind Borg, Erling Rytter, Anders Holmen*: Relation between methane, olefin and C_{5+} selectivity for cobalt based catalysts in Fischer-Tropsch synthesis*. In preparation
5. Sarka Zarubova, Shreyas Rane, Yingda Yu, Ye Zhu, De Chen, and Anders Holmen: *Structured Carbon Nanofibers-Carbon Felt composite: A Novel Support for Cobalt in Fischer-Tropsch synthesis*. In preparation.

Financial support:
The project is funded by The Research Council of Norway (NFR) through the GASSMAKS programme.

Microkinetic modeling of ethylene oxychlorination

Ph. D. student: Miroslav Surma.
Supervisor: Prof. De Chen

The oxychlorination of ethylene is an industrially important reaction catalysed by $CuCl_2/Al_2O_3$ and promoted with KCl. Although many kinetic models have been proposed, none of them is able to describe the reaction over a wide temperature interval. This is caused by quite complex reaction mechanisms in which different intermediates could occur.
Microkinetic modeling elucidates the reactions taking place on the catalyst surface. Many compounds being involved in the microkinetic model exist for only short period of time and/or are hardly visible by common characterization techniques. Thus, coupling of different techniques has to be used to get comprehensive data for further computational analysis. In situ IR, in situ Raman spectroscopy, TPD, TPSR, SSITKA and many others are popular methods for microkinetic data extracting.

The purpose of the project is to obtain a reliable microkinetic model to describe the oxychlorination of ethylene and link this model to reactor simulation. MATLAB is used as the computational enviroment for all simulations.
Moreover, a MATLAB application called "Easy Microkinetic Modeling", has been developed which should provide a simple evaluation of microkinetic models. The application overreaches the scope of the project and can be used for the microkinetic modeling of another processes.

Financial support:
The Research Council of Norway through the inGAP programme.

Understanding catalytic effects in Pd alloy model systems and membranes through advanced modelling.

Postdoctoral Fellow: Ingeborg-Helene Svenum
Supervisors: Associate Professor Hilde J. Venvik,
Professor Manos Mavrikakis, Univ. of Wisconsin

The manipulation of adsorption properties of catalysts and membranes in H_2/CO mixtures has been targeted many researchers, and has relevance to natural gas conversion in general and hydrogen technology in particular. We recently discovered that CO inhibition of hydrogen transport through PdAg membranes was significantly reduced by membrane heat treatment in air. Analysis by fitting of experimental data and modelling indicated changes in CO an H_2 heats of adsorption to be part of the picture. Surface spectroscopy indicated that surface segregation phenomena could be involved, but more investigations are needed to explain the effects.

The overall objective of this research is therefore to understand how the response of Pd alloy surfaces to carbon monoxide and carbon dioxide the in presence of hydrogen is affected by the structure and composition of the surface. Eventually, we wish to apply this knowledge to make improved membranes, membrane reactors and catalysts. This calls for application of advanced characterization techniques in conjunction with detailed calculations/modelling. A first approach is to apply density functional theory (DFT) calculations in order to determine preferred adsorption sites and bonding mechanisms of CO on Pd-Ag alloy surfaces. Dissociative adsorption of hydrogen will also be investigated in order to predict reaction pathways and activation energy barriers. The effect adsorbed CO has on the preferred dissociation pathways of hydrogen and energy barriers is targeted. The calculations are performed using the Dacapo code, which is a state-of-the-art planewave-pseudopotential implementation of DFT. The research is performed in a collaboration with Professor Manos Mavrikakis at University of Wisconsin-Madison, where Ingeborg-Helene Svenum is residing from Sept. 2009 through July 2010.

Financial support:
The research is funded by the Department of Chemical Engineering, NTNU and Statoil ASA through the NTNU-SINTEF Gas Technology Centre.

Insulating liquids

Ph.D. candidate: Ingvild Tronstad
Supervisors: Prof. Edd A. Blekkan, Marit-Helen G. Ese, SINTEF Energiforskning AS

High voltage transformers are isolated with mineral oil and solid cellulose (paper wrapt around the copper windings). Failures in these transformers have dramatic consequences for everyday life and industry. To prevent failures it is important to know how these insulating materials works in the transformer. By use of traditionally analysis methods, as titration, to new methods as QCM and microcalorimeter, we try to understand the reactions and effects of the chemicals in the insulating materials. With the focus on corrosion and formation of copper sulphide in transformer insulations and oxidation of insulating liquids including alternative, environment-friendly liquids, is this project a part of the KMB project "Thermal and electromagnetic performance of transformers". The KMB project is a joint project between Statnett, Hafslund, Statkraft, EDF, ABB, Nynäs, Siemens, NVE and the research counsil of Norway, where the work is done by SINTEF Energy research and NTNU.

Financial support:
Statnett, Hafslund, Statkraft, EDF, ABB, Nynäs, Siemens, NVE and The Research Counsil of Norway.

Deactivation of Cobalt based Fischer – Tropsch synthesis catalysts

Ph.D. candidate: Nikolaos Tsakoumis
Supervisor: Prof. Anders Holmen
Co-supervisors: Prof. II Erling Rytter and dr.ing Øyvind Borg, Statoil.

The Fischer-Tropsch synthesis is an important part of most natural gas conversion (GTL) process developments in recent years. Modern Fischer-Tropsch synthesis aims at converting synthesis gas into high quality diesel. A key element in improved Fischer-Tropsch technology is the development of active and stable catalysts with high wax selectivity. Cobalt is considered the most favourable metal for the synthesis of long-chain hydrocarbons.

Deactivation is an inevitable phenomenon in Fischer-Tropsch synthesis. Different mechanisms for catalyst deactivation have been proposed including re-oxidation of active sites, carbidization, polymeric surface carbon formation, sintering, metal support compound formation and surface reconstruction. Catalyst poisoning from impurities in the catalyst as well as from the feed may also result in catalyst deactivation.

The project aims at studying catalyst deactivation by different techniques. The main challenge for studying catalyst deactivation is the fact that the catalyst is embedded in wax after use. The wax, which is a main product, is limiting the range of techniques that can be used and the high sensitivity of the active phase against oxygen hampers the handling procedure. This leads to low reliability of the results that are obtained through a procedure involving sampling, dewaxing and characterizing at inert conditions. Thus, recent catalyst deactivation research has turned the attention to advanced *in-situ* (operando) characterization techniques. Proper selection of techniques will allow monitoring of the changes occurring inside the reactor during FTS and provide information that will assist in improved understanding of deactivation phenomena.

Achieving realistic FT conditions (200-400^{o}C, 20 bar, H_2/CO=2) with simultaneous data collection is very challenging. We have designed and constructed a modified Clausen type *in- situ* cell in order to combine photon based techniques and FT conditions at realistic conditions of temperature and pressure. The cell has successfully been tested at SNBL (ESRF, Grenoble). Several parameters have a pronounced influence on the FT catalyst deactivation, it is therefore important to involve several characterization techniques in order to distinguish the influence of external conditions and to identify the separate deactivation routes.

Publications and presentations in 2009:

1. Rønning, M., Voronov, A. S., Tsakoumis, N., Borg, Ø., Rytter, E., Holmen, A., *Decoupling of the deactivation mechanisms in Co-based Fischer-Tropsch catalysts by a wide range of in situ spectroscopies at realistic working conditions*, Oral Presentation, Operando III, Third International Congress on Operando Spectroscopy, 19-23 April 2009, Rostock-Warnemünde, Germany**.**
2. Tsakoumis, N., Borg, Ø., Rønnning, M., Rytter, E., Holmen, A., *Fischer-tropsch synthesis: in situ XRD study throughout reactions start-up,* Oral & Poster presentation, InGap–Nanocat Summerschool in Heterogeneous catalysis: Nano designed catalysts: from molecules to industrial processes, 21-26 June 2009, Trondheim, Norway.
3. Rønning, M., Voronov, A. S., Tsakoumis, N., Borg, Ø., Hammer, Nina, Rytter, E., Holmen, A., *Complimentary in situ characterisation techniques at realistic working conditions for the Fischer-Tropsch synthesis,* Oral Presentation, 14th International Conference on X-ray Absorption Fine Structure, 26-31 July 2009 Camerino, Italy.
4. Rønning, M., Tsakoumis, N., Voronov, A., Borg, Ø., Rytter, E., Holmen, A., *Deactivation studies of Co-Re/γ-Al2O3 Fischer-Tropsch catalyst.* Poster

presentation, EuropaCat IX: Catalysis for a Sustainable World, August 30 - September 4 2009, Salamanca, Spain.
5. Rønning, M., Tsakoumis, N., Voronov, A.S., Johnsen, R., Norby, P., van Beek, W., Borg, Ø., Rytter, E., Holmen, A., *Combined XRD and XANES studies of a Re-promoted Co/γ-Al_2O_3 catalyst at Fischer–Tropsch synthesis conditions*, Catalysis Today, doi:10.1016/j.cattod.2009.10.010.
6. Tsakoumis, N., Voronov, A. S., Borg, Ø., Rønning, M., Rytter, E., Holmen, A., *Deactivation studies on Re promoted Co/γ-Al2O3 catalysts for Fischer-Tropsch synthesis*, Poster presentation, 11th International Symposium on Catalyst Deactivation, 25 - 28 October 2009, Delft, The Netherlands.
7. Voronov, A.S., Tsakoumis, N., Borg, Ø., Rytter, E., Holmen, A., Rønning, M., *Deactivation studies of Co-based Fischer-Tropsch catalysts by in situ spectroscopies at realistic working conditions.* , Poster presentation, 11th International Symposium on Catalyst Deactivation, 25 - 28 October 2009, Delft, The Netherlands.
8. Tsakoumis, N., Voronov, A. S., Rønning, M., Borg, Ø., Rytter, E., Holmen, A., *Insights into catalyst deactivation phenomena in Co-based Fischer-Tropsch*, Poster presentation, Norwegian Catalysis Symposium 2009, November 30 - December 1 2009, Trondheim, Norway.
9. Voronov, A. S., Tsakoumis, N., Borg, Ø., Rytter, E., Holmen, A., Rønning, M., *Deactivation studies in Co-based Fischer-Tropsch catalysts*, Norwegian Symposium on Catalysis, November 30 - December 1 2009, Trondheim, Norway.

Financial support:
The project is funded by The Research Council of Norway through the inGAP programme and the Department of Chemical Engineering, NTNU.

Development of carbon nanostructured supports

Postdoctoral Fellow: Dr. Estelle Vanhaecke
Supervisors: Prof. Magnus Rønning, Prof. De Chen

Nanostructured materials are becoming increasingly important for many fields such as energy/storage tasks and also as potential catalytic supports. Recently a range of novel nanostructured catalytic materials were developed, which are now starting to be investigated in different applications in the area of energy conversion and storage. The common feature of these novel materials is to have a tailored nanoarchitecture based on a nanostructured alignement which offers different advantages such as improved charge transport (relevant to both electro- and photo-chemical devices); improved light harvesting and reduced light scattering and stable hybrid nanostructured oxide-carbon materials with an efficient electronic contact (relevant for both photo- and electro-chemical devices) to improve performances and kinetics in electrochemical energy storage.

The project focuses on the optimization of the catalytic CVD method to

synthesize aligned CNT as well as CNT/CNF layers on conductive substrates such as titanium, stainless steel, graphite and copper foils. The substrate is selected based on different applications and a Fe catalyst is introduced for in-situ CVD with organic metal compounds. Other supports such as carbon felt, sintered metal fibers are also used as nanostructured supports. Operation conditions including temperature, carbon sources, carbon to hydrogen ratio and growth time are studied to tune the CNT layer properties for each substrate.

The next step is to use these nanostructured reactors in various applications which can be nanocomposite development as supports for nanodots in solar cells and also as potential candidates in liquid reactions/filtration

Presentations in 2009:

1. Estelle Vanhaecke, De Chen, Fan Huang, *Nanostructured materials based on carbon nanostructures: candidate for solar cells*, oral presentation, Oppdal Workshop on PV Materials March 19-21th 2009
2. Estelle Vanhaecke, Fan Huang, De Chen, Magnus Rønning,*Carbon nanotubes Synthesis Composite on Foils*, oral presentation, Shinschu University, Beijing, seminar, March 2009
3. Estelle Vanhaecke, Fan Huang, De Chen, Magnus Rønning, *Aligned carbon nanotubes array, synthesis and applications in composite design for new energy and energy storage*, oral presentation, EuroNanoForum 2-5 June 2009, Prague
4. Estelle Vanhaecke, Fan Huang, De Chen, Magnus Rønning, *Carbon nanotubes Synthesis on Foils,* Statoil, Vista Scholar Day, invited presentation, 09 September 09
5. Estelle Vanhaecke, Fan Huang, De Chen, Magnus Rønning, *Carbon nanostructures synthesis on foils*, poster presentation, Norwegian Symposium on Catalysis, December 2009

Financial support:
NTNU strategic funding

Elaboration of carbon nanostructured reactors for catalytic water purification

Postdoctoral Fellow: Dr. Estelle Vanhaecke
Supervisors: Prof. Magnus Rønning, Prof. De Chen

The project deals with the preparation and testing of catalysts supported on structured reactors (ceramic and metallic honeycomb monoliths, metallic filters and carbon cloth) coated with nano-carbon materials (NCM), in the form of carbon nanofibers (CNF) and carbon nanotubes (CNT). The structured catalytic reactors will be used for catalytic water purification. The consortium will test the monoliths in various reactions focusing on different pollutants (Nitrates, organics) using a range of catalytic processes (hydrogenation, oxidation, ozonation) depending on the particular expertise of the partners.

The properties of the monolithic reactor coated with NCM, i.e. thin catalyst layer and mesoporosity, enable good control of the diffusion path and enhance the diffusion of reactants to the catalytic sites. The objective is to achieve an intensification of the catalytic processes in terms of improved selectivity, robustness, stability and performance while reduced energy requirements and by-product generation. This will realise advantages over conventional reactors, such as trickled bed reactors or slurry reactors.

Objectives
Process intensification of catalytic water treatment. Preparation of materials with control of the structure at different length scales (from nm to m). Knowledge transfer between experts in coating, catalyst preparation, process design and end users for water treatment

Partners in the consortium
Instituto de Carboquímica-CSIC, Zaragoza – ES
Norwegian University of Science and Technology – NO
Universidad Politécnica de Valencia – ES
Faculdade de Engenharia da Universade do Porto – PT
Norta – LT
University of Warwick – UK
MEL chemicals, a division of magnesium elektron limited – UK
VEOLIA – FR
Ecole Polytechnique Fédérale de Lausanne - CH

Presentations in 2009:

1. Estelle Vanhaecke, Fan Huang, De Chen, Magnus Rønning,*Carbon nanotubes Synthesis Composite on Foils*, oral presentation, Shinschu University, Beijing, seminar, March 2009
2. Estelle Vanhaecke, Fan Huang, De Chen, Magnus Rønning, *Aligned carbon nanotubes array, synthesis and applications in composite design for new energy and energy storage*, oral presentation, EuroNanoForum 2-5 June 2009, Prague
3. Estelle Vanhaecke, Fan Huang, De Chen, Magnus Rønning, *Carbon nanostructures synthesis on foils*, poster presentation, Norwegian Symposium on Catalysis, December 2009

Financial support:
Monacat Project, EU,FP-7 programme
Grant Agreement n^{o} 226347
www.monacat.eu

Study of the deactivation mechanisms inCo-based Fischer-Tropsch catalysts at realistic working conditions

Ph.D. candidate: Alexey Voronov
Supervisor: Prof. Magnus Rønning

The Fisher-Tropsch (FT) synthesis is the central step in gas-to-liquid (GTL) technology where H_2 and CO is converted into synthetic crude oil. The hydrocarbons produced in this step are paraffins and olefins with different carbon chain lengths. Due to low water-gas-shift activity, supported cobalt catalysts are often selected as functional materials for the FT synthesis from natural gas.

Nevertheless these catalysts are exposed to several deactivation mechanisms such as active phase transformation, carbon species deposition, surface reconstruction, sintering and cobalt reoxidation. An important challenge is to characterize and describe the individual steps and processes which take place on the catalyst surface during reaction.

Since there is no direct method to monitor the behaviour of the Co particles on the support surface, it is essential to apply several characterization techniques in order to distinguish the influence of the various external conditions and define the individual deactivation mechanisms. Investigation at realistic working conditions is necessary to obtain reliable data about the processes which occur on the catalyst during FT reaction.

So far, techniques such as XRD, XAS, TGA and Raman spectroscopy have been used. A number of parameters have a significant influence on the FT catalyst deactivation. Thus, it is essential to involve several characterization techniques in order to identify the ifluence of the various external conditions and define the separate deactivation routes.

The purpose of the project is to get detailed information about deactivation mechanisms and the effect of reaction conditions which may lead to new insight in catalyst formulation for FT synthesis in commercial GTL technology.

Publications and presentations in 2009:

1. M. Rønning, N.E. Tsakoumis, A.S. Voronov,R. Johnsen, P. Norby, W. van Beek, Ø. Borg, E. Rytter, A. Holmen. *"Combined XRD and XANES studies of a Re-promoted Co/γ-Al2O3 catalyst at Fischer–Tropsch synthesis conditions,"* Catalysis Today, doi:10.1016 /j.cattod.2009.10.010.
1. A. Voronov, Ø. Borg, E Rytter, A. Holmen, M. Rønning. *Deactivation studies of Co- based Fischer-Tropsch catalysts by in situ spectroscopies at realistic working conditions.* Poster. InGap Nanocat-III summer school, Trondheim, Norway, June 21-26, 2009.
2. A. Voronov, N.E. Tsakoumis, Ø. Borg, E Rytter, A. Holmen, M. Rønning. *Deactivation studies of Co- based Fischer-Tropsch catalysts by X-ray absorption spectroscopy at realistic working conditions.* Poster. International Symposium on catalyst deactivation, Delft, Netherlands, October 25-28, 2009.

3. Alexey Voronov, Nikolaos E. Tsakoumis, Øyvind Borg, Erling Rytter, Anders Holmen, Magnus Rønning. *Deactivation studies in Co-based Fischer-Tropsch catalysts.* Oral presentation. Norwegian symposium on catalysis, November30-December 1, 2009

Financial support:
The project is funded by NTNU and The Research Council of Norway through the inGAP programme.

Kinetic study of methane steam reforming over hydrotalcite based Ni catalyst modified by different metals

Postdoctor fellow: Dr. Hongmin Wang
Supervisor: Prof. De Chen, Prof. Anders Holmen

Methane steam reforming is an established technology for large scale hydrogen production in chemical industry. It combined with water gas shift reaction and a preferential oxidation reaction or pressure swing adsorption can produce very pure hydrogen. However, this process is complicated and costly. The exploration of advanced technologies for hydrogen production from nature gas has attracted greatly research interests in recent years. This project proposed a novel concept of hydrogen generation with CO_2 capture in a two stage methane steam reforming high temperature membrane reactor. The current study is a part of this project, which aims to design an improved nickel catalyst to reduce carbon formation**.** To aid in search for this catalyst, we seek an improved understanding of the processes occurring on the catalyst surface. DFT calculation indicates addition of transition metals on the Ni surface can destabilize intermediates leading to surface carbon formation, and thus improve the catalyst stability. A series of hydrotalcite-based Ni catalysts modified by different loadings of transition metals of Ag, Rh, Pt, and Pd were prepared by surface redox reaction. The catalysts were characterized by many different techniques such as TPR, XRD, TEM and XPS. The effect of surface alloying of Ni catalysts by different metals on the kinetic activity and carbon formation was studied by using methane steam reforming as a probe reaction. The activity test indicates that methane steam reforming reaction rates over the catalysts modified by different metals show the trend of Rh>Ni>Pt>Pd. The results of this study are helpful for the design of a high performance catalyst for methane steam reforming.

Presentations in 2009:

1. Hongmin Wang, Anh H. Dam, D. Wayne Blaylock, Teppei Ogura,Yian Zhu, Anders Holmen, William H. Green, and De Chen, *Kinetic study of methane steam reforming over Ni catalyst modified by silver designed by*

first principle, International Symposium on Relations between Homogeneous and Heterogeneous Catalysis, 13-18 September 2009, Stockholm, Sweden.

2. Hongmin Wang, Anh H. Dam. Wayne Blaylock, Teppei Ogura,Yian Zhu, Anders Holmen, William H. Green, and De Chen*, Kinetic study of methane steam reforming over Ni catalyst modified by silver*, 1st Trondheim Gas technology conference, 21-22, October, 2009, Trondheim, Norway.
3. Hongmin Wang, Anh H. Dam, D. Wayne Blaylock, Teppei Ogura,Yian Zhu, Anders Holmen, William H. Green, and De Chen, *Kinetic study of methane steam reforming over hydrotalcite-based Ni catalyst modified by different metals,* Norwegian catalysis symposium 2009, 30/Nov-01/Dec, 2009, Trondheim, Norway.

Financial support:
The Research Council of Norway

Advanced Cleaning Devices for Production of Green Syngas

Postdoctoral Fellow: Dr. Espen S. Wangen
Supervisor: Professor Edd A. Blekkan

The production of fuels from biomass may become important in the effort of reducing greenhouse gas emissions to the atmosphere. Biofuels may be synthesised through a thermochemical process route, involving biomass gasification to produce synthesis gas (syngas) as the intermediate product. The conditioning of such a gas will be challenging, as it contains large amounts of contaminants. The gas cleaning will involve several steps, e.g. removal of alkali metals and particulates, sulphur (COS, H_2S), and ammonia. Higher hydrocarbons, tars, may cause problems due to condensation and plugging of pipes and processing units, and need to be removed.

The Catalysis group participates in the project "Advanced Cleaning Devices for Production of Green Syngas" (GreenSyngas), funded by the European Commission under its 7th Framework Program. The consortium consists of 10 partners from both industry and academia. The aim of the project is to develop a novel gas conditioning process to clean the raw product gas from a wood gasification plant. The plant is located in Güssing, Austria. The quality of the conditioned syngas should meet the requirements for a feedstock used in the production of vehicle fuels.

The task of the Catalysis group is the reforming of unconverted hydrocarbons in the raw product gas from gasification. In addition, studies on the water gas shift reaction will be carried out. The focus of the studies will be reaction kinetics, catalyst stability and deactivation.

Project webpage: http://www.eat.lth.se/greensyngas/

Publications and presentations in 2009:

1. E. S. Wangen, A. Malik, M. Sanati, E. A. Blekkan*: On the steam reforming of producer gas in the production of clean bio-syngas*. Oral presentation. Norwegian Symposium on Catalysis. Trondheim (Norway), November 2009 .
2. E. S. Wangen, K. R. Trehjørningen, L. He, D. Chen, E. A. Blekkan. *Reforming raw synthesis gas from wood gasification.* 21st North American Catalysis Society Meeting, San Francisco (USA), June 2009.
3. Malik, J. Pagels, E. Wangen, M. Lindskog, E. Blekkan, M. Sanati. *Investigation of catalyst deactivation by deposition of size selected soot particles*. Poster presentation. Nordic Aerosol Conference, Lund (Sweden), November 2009.

Financial support:
The project is funded by the European Commission under its 7th Framework Program, and co-financed by the Swedish Energy Agency.

Steady-State Isotopic Transient Kinetic Analysis (SSITKA) of Catalytic Reactions

Ph.D. candidate: Jia Yang
Supervisors: Prof. Anders Holmen, Prof. De Chen

Steady-state isotopic transient kinetic analysis (SSITKA) has proved to be a powerful technique for studying heterogeneous catalyzed reactions. By normal steady-state experiments only the overall reaction rate, i.e. the product of the rate constant and the site coverage, is determined. SSITKA combines both the steady-state and the transient technique and makes it possible to study the intrinsic reaction rate at the active catalytic site decoupled from the site coverage. The method can also be used to study details of the surface reactions such as single or multiple pools of reaction intermediates on the catalytic surface and the reactivity distribution within the pools. A SSITKA experiment consists of making a switch between different isotopic labeled reactant species, such as ^{12}CO and ^{13}CO. The feed for example ^{12}CO-H_2 or ^{13}CO-H_2, is converted at steady-state over the catalyst provided that no isotopic effect occurs, and the transient response after the switch is monitored by a mass spectrometer. The focus so far has been on the production of fuels from natural gas by the Fischer-Tropsch synthesis on Cobalt catalysts. The activity and selectivity depend on the crystal size for small Cobalt particles, and SSITKA has contributed to the detailed understanding of the mechanism. The experiments have recently been expanded to include $C^{16}O$ and $C^{18}O$ as well as $^{16}O_2$ and $^{18}O_2$. The oxygen switches are particularly interesting for oxidation reactions on solid surfaces.

Publication and presentations in 2009:

1. J.P. den Breejen, A.M. Frey, J. Yang, A. Holmen , M.M. van Schooneveld, O.Stephan, J.H. Bitter K.P. deJong,: *Highly active and selective manganese oxide promoted cobalt-on-silica Fischer-Tropsch catalysts.* (to be submitted)
2. J. Yang, E.Z. Tveten, Ø. Borg, E. Rytter, A. Holmen: *Effect of Support and Metal Particle Size on the Intrinsic Activity and Selectivity for Co-based Fischer-Tropsch Catalysts.* Oral presentaion. Norwegian Catalysis Symposium 2009, Trondheim, Norway. November 30 – December 1, 2009.
3. J. Yang, E.Z. Tveten, Ø. Borg, E. Rytter, A. Holmen: *Effect of support on the Intrinsic Activity and Selectivity for Co-based Fisher-Tropsch Catalyst*. Poster. EuropaCat IX, Salamanca, Spain August 30 - September 4, 2009.
4. Xuyen Kim Phan, Jia Yang, Hamidreza Bakhtiary, R. Myrstad, H.J. Venvuk, A. Holmen: *Studies of Macroporous Structured Alumina based Cobalt Catalysts*. Poster. EuropaCat IX, Salamanca, Spain August 30 - September 4, 2009.

Financial support:
The project is funded by The Research Council of Norway (NFR), through the "KOSK" program.

Novel structured reactor for CO removal

Postdoctoral Fellow: Dr. Tiejun Zhao

Supervisor: Prof. Magnus Ronning

In this project, we focus on the fabrication of novel structured reactors for CO removal in H_2 rich feed, aiming at obtaining fuel cell quality H_2. Cu-CeO_2 nanocomposite and Cu-CeO2 supported on structured carbon nanofibers (sCNF) are prepared and tested.

Preferential oxidation (PrOx) has been recognized as one of the most straightforward and cost-efficient methods to achieve acceptable CO concentrations (mostly below 10 ppm) during H_2 production in low-temperature proton-exchanged membrane fuel cell applications. During the last decade, the ability of supported noble metal catalysts, in particular containing platinum and gold have been demonstrated for the PrOx reaction. Special attention has been devoted to the catalysts based on Cu-CeO_2, which exhibit higher selectivity than Pt metal supported catalyst at similar CO conversion levels and considerably higher stability than the Au-containing catalysts.

In this project, a structured carbon nanofiber supported Cu-CeO_2 catalyst has been developed by impregnation of the Cu-Ce-citrate complex solution onto the oxidized structured carbon nanofiber/carbon felt composite support, before calcination at 673 K. For comparison, the powder Cu-CeO_2 nanocomposites are prepared by a similar method. The structured catalyst formed is characterized by TGA, BET, XRD, TPR, SEM, HRTEM, showing that the Cu-CeO_2

nanoparticles are mostly deposited on the surface of structured carbon nanofibers. Both the nanocomposite and the structured catalysts are tested in the preferential oxidation of CO in hydrogen rich gases. A higher activity and selectivity to CO oxidation is achieved on the Cu-CeO_2/sCNF compared to the powdered nanocomposites. This is due to the smaller particle size of Cu-CeO_2 and the high thermal conductivity of the carbon nanofibers.

Publications and presentations in 2009

1. Tiejun Zhao, Yingda Yu, Xiaofeng Yu, Steinar Raaen, De Chen, Magnus Ronning. *Peferential oxidation of CO in H2-rich gases over the Pechini-methodderived Cu-CeO2 nanocomposite and monolith catalysts,* Aug. 13-15, 2009 China-North America Workshop on Fuel Cell Science and Technology, Oral presentation.
2. S. Boullosa-Eiras, T. Zhao, Y. Yu, D. Chen, A. Holmen. *Supported Rh on ZrO2-Al2O3 nanocomposite catalyst for catalytic partial oxidation of methane to syngas.* Poster presentation. 6th World Congress on Oxidation Catalysis, 5-10 July 2009, Lille, France.
3. T. Zhao, S. Boullosa-Eiras, Y. Yingda, Y. Xiaofeng, S. Raaen, M. Ronning, D. Chen, A. Holmen. *Synthesis and catalytic performance of high-temperature stable nanocomposites by a versatile nanoparticle-mediated Pechini method.* Oral presentation. EuropaCat2009, 30 August – 4 September 2009, Salamanca, Spain.
4. S. Boullosa-Eiras, T. Zhao, E. Vanhaecke, Y. Yu, D. Chen, A. Holmen. *Ce-Zr-Al mixed oxide nanocomposites supported Rh: a promising catalyst for partial oxidation of methane to syngas*. Poster presentation. Norwegian catalysis symposium 2009, 30 November – 1 December 2009, Trondheim, Norway.
5. S. Boullosa Eiras, T. Zhao, Y. Yu, D. Chen, A. Holmen. *Alumina-based nanocomposite supported Rh catalysts: an effective and highly stable catalyst for partial oxidation of methane to syngas*. Poster presentation. EuropaCat2009, 30 August – 4 September 2009, Salamanca, Spain.
6. Tiejun Zhao, Yingda Yu, De Chen, Magnus Ronning, *Carbon nanofiber/carbon felt supported Cu-CeO2 catalyst: a promising structured catalyst for preferential oxidation of CO in H2- rich gases,* Poster presentation. Norwegian catalysis symposium 2009, 30 November – 1 December 2009, Trondheim, Norway.
7. Kvande, I.; Chen, D.; Zhao, T. J.; Skoe, I. M.; Walmsley, J. C.; Ronning, M. *In Hydrogen Oxidation Catalyzed by Pt Supported on Carbon Nanofibers with Different Graphite Sheet Orientations*, Topics in Catalysis, 2009; 52, 664-674.
8. Li, P.; Huang, Y. L.; Chen, D.; Zhu, J.; Zhao, T. J.; Zhou, X. G., **CNFs-supported Pt catalyst for hydrogen evolution from decalin.** Catalysis Communications 2009, 10, (6), 815-818.
9. Ochoa-Fernandez, E.; Zhao, T. J.; Ronning, M.; Chen, D., *Effects of Steam Addition on the Properties of High Temperature Ceramic CO2*

Acceptors. Journal of Environmental Engineering-Asce 2009, 135, (6), 397-403.
10. Zhu, J.; Zhou, J. H.; Zhao, T. J.; Zhou, X. G.; Chen, D.; Yuan, W. K., *Carbon nanofiber-supported palladium nanoparticles as potential recyclable catalysts for the Heck reaction*. Applied Catalysis A:General 2009, 352, (1-2), 243-250.
11. Tiejun Zhao, Yingda Yu, Magnus Ronning, *Carbon nanofiber/carbon felt supported Cu-CeO2: a promising structured catalyst for preferential oxidation of CO in H2-rich gases*, to be submitted.

Financial support

The Research Council of Norway (NFR), KOSK programme

Engineering of Pt nanoparticles in Propane Dehydrogenation

Postdoctoral Fellow: Dr. Jun Zhu
Supervisor: Prof. De Chen

Catalytic dehydrogenation of NGL compounds (ethane, propane, butane) is an important industrial process. Although they have been extensively studied, a complete understanding of reactions on the catalyst surface including selectivity, coke formation and deactivation is still missing. Nanocrystals of different size of noble metals are attractive for use as catalysts because of their different surface-to-volume ratios and high surface area, which in turn cause their surface atoms to be highly active. Meanwhile, nanocrystals of shape control could enable the properties of a nanocrystal to be tuned with a greater versatility than can be achieved otherwise. In this sense, it is of great interest to investigate the effects of different Pt surface atoms on the dehydrogenation reactions.
The project is aimed in that it 1) explores the novel Pt based nanoparticles with well controlled shapes and sizes towards catalysts with better activity and good stability in propane dehydrogenation (DHP), 2) focuses on the fundamental study of the catalyst structure-properties-performance relationship 3) improves the ability in rational design of catalysts in heterogeneous catalysis.

Up to now, different size and shape of Pt nanoparticles, which have different ratio of surface sites on the surface and varied in the orientations of the surface such as {111}, {100}, have prepared and characterized by XRD, SEM and HRTEM. These Pt nanoparticles were supported on Mg(Al)O, a calcined hydrotalcite with high surface area (typical 160-220 m2/g) and a basic character. The effects of surface atoms and facets of Pt nanoparticles on the activity, selectivity and coking in DHP have been investigated for the first time. The catalytic performance indicates a strong structure-sensitive character. The aparent activation energies of dehydrogenation and hydrolysis on different Pt facets, {111} and {100}, edges and corners vary a lot, which result in different

catalytic activity and selectivity. Moreover, the coke formation is also a structure sensive reaction on Pt catalysts. Pt nanoparticles with smaller particles size are more active for coke formation and have lower stability.

It will be important to prepare different size of well-controlled shape of Pt nanoparticles and characterize these catalysts with extended methods, such as HRTEM, EXAFS, XANE, Raman, TPR, etc. The catalysts are to be improved according to the structure activity/selectivity/stability relationships.

Publications and presentations in 2009:

J. Zhu, M. Rønning, Y. Yu, A. Holmen, D. Chen : *Platinum nanoparticle shape effect onpPropane dehydrogenatio*n, Norwegian Symposium on Catalysis 2009, Oral presentation.

Financial support:

The Research Council of Norway (NFR).

SINTEF Projects

Preparation of alumina support for Fischer-Tropsch catalysis by spray-drying

Staff: Dr. Anna Lind, Siv.ing. Rune Myrstad

Porous alumina particles, that are to be used as support in Fischer-Tropsch catalysis, have been produced by spray drying of alumina primary particles. The alumina material is formed by agglomeration of the primary particles during the spray drying process. We have investigated the influence of both instrumental parameters, as well as the condition of the suspension of primary particles on the porosity, as well as the particle size and morphology of the materials. Some of the materials have also been impregnated with cobalt and rhenium by the incipient wetness method and tested in a fixed bed reactor.

Publications and presentations:

1. A. Lind, A. Holmen, R. Myrstad, S. Eri, T. Hulsund Skagseth, E. Rytter: *Spray Drying of Porous Alumina Support for Fischer-Tropsch Catalysis*, submitted to Studies in Surface Science and Catalysis, under review.
2. T. Noor, A. Lind, A. Holmen, D. Chen: *Synthesis and Characterization of Nickel Hydrotalcite Catalyst for Hydrogen Production Using the Co-Precipitation, Spray Drying and Microemulsion Method*. Poster. Norwegian Catalysis Symposium 2009, Trondheim, Norway, November 30-December 1, 2009.
3. A. Lind, A. Holmen, S. Eri, T. Hulsund Skagseth, E. Rytter: *Spray Drying of Porous Alumina Support for Fischer-Tropsch Catalysis*. Poster. Norwegian Catalysis Symposium 2009, Trondheim, Norway, November 30-December 1, 2009.

Client: The Research Council of Norway through the inGAP programme.

An Integrated Process for Hydrogen Production and Separation

Project category: A used directed project with StatoilHydro as industrial partner (RENERGI-BIP, 2008-2011), including cooperation with IFE and NTNU (PhD) on hydride materials.

Staff (SINTEF Materials and Chemistry): Senior scientist Rune Lødeng & Scientist Svatopluk Chytil (Dept. Process Technology - Catalysis), Senior Scientist Yngve Larring (Dept. Energy conversion and materials), Scientist Bjørnar Arstad and Scientist Marit Stange (Dept. Process chemistry).

Main goal
The aim of the project is to combine two novel technologies in order to achieve a highly efficient process for hydrogen production from carbon containing fuels. The two processes are: i) Catalytic partial oxidation by lattice oxygen from oxide based materials, and ii) Sorption enhanced conversion of CO and C_2H_5OH by integration of the water gas shift (WGS) and reforming reactions with hydrogen absorbing materials.

CPO (The SINTEF activity)

One objective is to develop new catalyst materials, with an ability to provide oxygen from the crystal lattice or grain boundaries to the oxidation/reforming reactions. Scientific challenges are particularly focused on development of heterogeneous carriers and catalysts, and improved utilization of different oxygen types (lattice oxygen, surface oxygen, near surface oxygen, grain border oxygen, etc). Other important issues that will be addressed include the interplay between carriers and a metal function, oxygen storage and release properties. Major challenges on a short-term are:

- Investigations of different oxygen types, their properties and availability to reactants.
- Understand selectivity governing factors as a basis for innovation.
- Identify promising materials that can be used for tuning the availability of O_2 types.
- Use of non-oxygen containing carriers in combination with an active phase.
- Optimization of catalytic oxidation properties at moderate temperature to produce the required heat at the right place.
- Catalyst stability at high temperature.
- Effect of presence of steam.

Candidate materials have been synthesised in Oslo and tested in Trondheim.

Funding: Statoil and the Research Council of Norway (RENERGI)

Dehydrogenation of propane over chromium oxide based catalysts

Staff: Prof. Chen De, Prof. Anders Holmen (Dept. Chem. Eng. – NTNU), Senior scientists Rune Lødeng and Magne Lysberg (SINTEF Materials and Chemistry, Dept. Process Technology).

Kinetic data for the main PDH reaction and the carbon formation has been obtained in the tapered element oscillating microbalance reactor and applied for building kinetic models. A number of candidate commercial catalysts have been

investigated and benchmarked. Predictive modeling of an industrial plant performance was part of the project work earlier. Development of reactor models is part of ongoing work.

Client: Borealis Polyolefine, Linz – Austria

Improved Fischer-Tropsch catalysts

Staff: Siv.ing. Rune Myrstad and Ing. Odd Asbjørn Lindvåg: SINTEF, Prof. Anders Holmen and Prof. Edd Anders Blekkan: NTNU

The goal of this project is to support the clients' development of catalysts for the Fischer-Tropsch synthesis by testing and characterization of catalysts.

Publications and presentations in 2009:

1. B.C. Enger, O. Borg, A.L. Fossan, O.A. Lindvag, R. Myrstad, S. Eri, E. Rytter, A. Holmen: *Fischer-Tropsch synthesis on Co supported on modified alumina,* Abstract of Papers of the American Chemical Society, 236 (2008)
2. Ø. Borg, N. Hammer, S. Eri, O.A. Lindvåg, R. Myrstad, E.A. Blekkan, M. Rønning, E. Rytter, A. Holmen: *Fischer-Tropsch synthesis over un-promoted and Re-promoted γ-Al_2O_3 supported cobalt catalysts with different pore sizes*, Catalysis Today. 142 (2009) 70-77

Client: Statoil R&D

Study of Fischer-Tropsch Synthesis in a microstructured reactor

Staff: Siv.ing. Rune Myrstad and Ing. Odd Asbjørn Lindvåg: SINTEF, Prof. Anders Holmen: NTNU

Microstructured reactor technology is an emerging technology for the Fischer-Tropsch synthesis (FTS). The goal of this project is to investigate the microstructured reactors potential for FTS and verify claims from technology providers. A microstructured reactor for FTS is fabricated at Karlsruhe Institute of Technology and its performance on FTS is tested and evaluated.

Publications and presentations in 2009:

1. R. Myrstad, S. Eri, P. Pfeifer, E. Rytter, A. Holmen, *Fischer-Tropsch synthesis in a microstructured reactor,* Lecture. EuropaCat IX, Salamanca, Spain, September, 2009
2. R. Myrstad, S. Eri, P. Pfeifer, E. Rytter, A. Holmen, *Fischer-Tropsch synthesis in a microstructured reactor,* Lecture. ICOSCAR-3, Ischia, Naples, Italy, September, 2009

3. R. Myrstad, S. Eri, P. Pfeifer, E. Rytter, A. Holmen, *Fischer-Tropsch synthesis in a microstructured reactor*, Catalysis Today. 147 (2009) S301-S304.
4. R. Myrstad, S. Eri, P. Pfeifer, E. Rytter, A. Holmen, *Fischer-Tropsch synthesis in a microstructured reactor,* Lecture. Norwegian Symposium on Catalysis, Trondheim Norway, November 2009

Client: The Research Council of Norway through the InGAP programme.

Compact gas to products technology

Staff: Siv.ing. Rune Myrstad, SINTEF, Prof. Anders Holmen and Assoc. prof. Hilde J. Venvik: NTNU.
Ph.D. Candidates: Hamidreza Bakhtiary and Xuen Kim Phan

The goal of this project is identification and evaluation of concepts for micro structured reactors, enabling compact and efficient offshore gas to products technology with main focus on the methanol synthesis (throughput and selectivity).

The project is a part of the KMB (Competence building with user involvement)-project "Enabling production of remote gas" under Petromaks (Solutions for remote gas) program in the Research Council of Norway.

Through a coordinated effort by industry and research institutions, the KMB-project will address challenges related to critical technology barriers concerning floating production of natural gas from remote fields. Specific challenges are: Safety, reliability, process equipment movement, weight and compactness combined with robust operation.

Publications and presentations in 2009:
1. H. Bakhtiary D., F. Hayer, X. K. Phan, R. Myrstad, H.J. Venvik, P. Pfeifer, K. Schubert, A. Holmen: *Methanol Synthesis in a Micro Packed Bed Reactor – Heat Exchanger.* Lecture. North American Catalysis Society Meeting, San Francisco, USA, June, 2009.
2. X. K. Phan, H. Bakhtiary D., R. Myrstad, J. Thormann, P. Pfeifer, H.J. Venvik, A. Holmen: *Studies of Macroporous structured Alumina based Cobalt Catalysts*, Poster presentation at Europacat IX, Salamanca, Spain, September, 2009
3. H. Bakhtiary D., F. Hayer, X.K. Phan, R. Myrstad, P. Pfeifer, H.J. Venvik, A. Holmen: *Methanol synthesis from syngas in a short contact time microstructured reactor*, Poster presentation at Norwegian Symposium on Catalysis, Trondheim, Norway, November, 2009
4. X.K. Phan, H. Bakhtiary D., R. Myrstad, J. Thormann, P. Pfeifer, H.J. Venvik, A. Holmen: *Experimental Study of Methanol Synthesis in a $PdCeO_2$*

Stacked Microchannel Reactor, Poster presentation at Norwegian Symposium on Catalysis, Trondheim, Norway, November, 2009

Client: The Research Council of Norway.

Refinery operations / Octane processes

Staff: Dr.ing. Torbjørn Gjervan, Ph.D. Ingvar Kvande and Ing. Merete Wiig

The project aims to improve the performance of the client's commercial catalytic reforming and isomerisation units. This includes catalyst evaluations, process optimization, general trouble-shooting and education of refinery personnel. The heart of the project is a small-scale pilot unit, but additional chemical or physical characterization tools are used as well.

Client: Statoil R&D

Hydrotreating

Staff: Dr.ing. Håkon Bergem, Ing. Camilla Otterlei, SINTEF. Prof. Edd A. Blekkan, NTNU

The project aims to improve the performance of the client's commercial hydrotreating units. New fuel specifications and changing crude oil qualities call for continuous development of existing and new refinery processes. We are involved in research aiming at developing new and better catalysts but also process optimization and modeling based on insight into the detailed mechanisms of the actual reactions. The processes are studied in bench- and pilot scale reactors.

Publications and presentations in 2009

1. H. Bergem, C. Otterlei, E.A. Blekkan, B. Thorvaldsen, P.A. Skjølsvik, B. Seljestokken. J.S. Rosvoll: *The effect of organic nitrogen compounds on gas oil hydrodesulfurization studied in a pilot plant.* Lecture. EuropaCat IX, Salamanca, Spain, September 2009.

Client: Statoil R&D

Ph.D. Theses in 2009

Astrid Lervik Mejdell: *Properties and application of 1-5 µm Pd 23wt.% Ag membranes for hydrogen separation*

Master (Diploma) Students in 2009

Inger Lise Bjørn: *Characterization of products from conversion of heavy oils*.

Ragnhild Høyen: *Characterization of alumina supported cobalt based catalysts*

Kathrine Storsæter*: Optimalization of the polymerization process at the Mongstad refinery.*

Kristin Rem Trehjørningen: *Biomass gasification*

Rafael Vera Lozadra: *Characterization of crude oils according to corrosivity using the Fe Powder test.*

Elisabeth Winstad*: Advanced characterization of Fischer-Tropsch catalysts.*

Xi Zhang: *Design, synthesis and characterization of bimetallic catalysts*

Christina Azpeleta Noiega: *Partial oxidation of methane by chemical looping.*

Group meetings with seminars 2009

Location: Kromaten, SINTEF

Schedule	Time	Presenter	Topic
February 20	1300	Kolbjørn Zahlsen SINTEF Bioteknologi	Mass spectrometry in chemical engineering? Possibilities and cooperation
March 6	1400	Jia Yang	An introduction to Steady-State Isotopic Transient Kinetic Analysis
March 20	1400	Tiejun Zhao	Preferential Oxidation of CO in H_2-rich gases over Cu-CeO_2 catalysts: Prospects and Progress
March 27	1400	Espen Standal Wangen	On the Thermochemical Conversion of Biomass to Syngas: Prospects and Progress
April 17	1400	Olaf Köhler Chemspeed Technologies AG	High-output experimentation - automation as an invaluable tool in the development of heterogeneous catalysts
May 29	1400	No presentation	

Schedule	Time	Presenter	Topic
August 21	1400	Li He	Approaching efficient production of hydrogen from biomass
September 11	1400	Wayne Blaylock	MIT Density functional theory calculations - basic principles and results
September 25	1430	Rune Myrstad SINTEF MK	Fischer-Tropsch synthesis in a microstructured reactor
October 9	1400	Christine Balonek Department of Chemical Engineering, University of Minnesota	Millisecond Catalytic Reforming of Solid Polymers: Polystyrene Monoaromatic Representatives over Noble Metals.
October 23	1400	Miroslav Surma	Algorithmization of some microkinetic issues
November 6	1400	Daham Gunawardana IKP NTNU/Kyungpook National University, South Korea	Copper-ceria catalysts for water gas shift and (oxidative) steam reforming of methanol.
November 20	1400	Oana Mihai	The volatility properties of reformulated gasolines with alcohols
December 4	1400	Hongmin Wang	Fuel cell basics

TKP4110 Chemical Reaction Engineering

Coordinator:
Professor Anders Holmen

Lecturers:
Professor Anders Holmen, Assoc. Professor Jens-Petter Andreassen,
Professor Heinz Preizig (laboratory exercises)

Semester: Fall

Level: 3th year

Credits: 7.5 SP

Course Plan:
Lectures (4 h/week), exercises (6 h/week), self study (2 h/week)

Objectives:
The course deals with the design of chemical reactors based on the reaction kinetics and the physical conditions in the reactor

Prerequisites:
The course is based on the compulsory courses at the Faculty of Chemistry and Biology, but students from other faculties may take the course as well, possibly after an introductory self-study.

Contents:
The course is divided in a theoretical part and a laboratory part. The theoretical part contains an overview of homogeneous and heterogeneous reaction mechanisms with particular emphasis on the relation between diffusion, heat transfer and reaction rate. Heterogeneous catalysis including reactions between gases, liquids and solid materials is also dealt with. Calculation of conversion and yields in batch reactors and in flow systems i.e. plug flow reactors and continuous-stirred tank reactors. Reactor stability and optimization of the reaction path. The laboratory work includes one exercise related to a topic from the theoretical part.

Teaching form:
The course is given as a combination of lectures, exercises, self-study and laboratory work. Admission to the exam requires that ½ of the exercises are approved. The theoretical part counts for 75% and the laboratory part for 25% of the final mark. Both parts must be passed in order to pass the course.

Course material:
H. Scott Vogler: Elements of Chemical Reaction Engineering. Prentice-Hall, Inc. 4rd ed., 2006.

Exam: Written + exercises

TKP4120 Process technology

Responsible:
Professor Edd A. Blekkan

Lecturers:
Professor Edd A. Blekkan

Semester: Fall

Level: 2nd year

Credits: 7.5 SP

Restricted admission: No

Course Plan:
4 lectures, 4 hours exercises and 4 hours self study per week

Goal:
The course gives an introduction to the process industry, and provides tools for quantitative calculations and modeling of processes, including mass- and energy balances, and chemical equilibrium calculations.

Prerequisites: None

Contents:
Topics from thermodynamics and physical chemistry: State variables, ideal gas, equations of state, work and heat, Laws of thermodynamics, entropy, Gibbs energy, equilibrium. Topics from process engineering: The balance principle. Mass balances. Mass balances with chemical reactions. Energy balances (2nd law of thermodynamics). Heat exchange. Mechanical work (compression and expansion). Work from heat. Mechanical energy balances.

Teaching form/language:
Lectures (in Norwegian), compulsory exercises and project work

Course material:
S. Skogestad, Prosessteknikk, Tapir Akademisk Forlag 2000.

Exam: Written (4 hours)

TKP4150 Petrochemistry and oil refining

Responsible:
Professor Edd A. Blekkan

Lecturers:
Professor Edd A. Blekkan, Professor II Kjell Moljord (Statoil), and Assoc. Professor Hilde J. Venvik, Professor Anders Holmen

Semester: Spring

Level: 4th year.

Credits: 7.5 SP

Restricted Admission: No

Course Plan:
3 Lectures, 2 hours exercises and 7 hours self study and projects per week.

Objective:
To provide an overview of the central processes for the conversion and upgrading of oil and natural gas.

Prerequisites:
Basis chemistry and mathematics and course TKP4155 Reaction Kinetics and Catalysis or similar knowledge.

Contents:
Feedstocks, Norwegian oil and gas production, energy from fossil fuels. Oil refining, oil products, refinery design and selected processes, catalytic reforming and isomerization, hydrotreating and hydrocracking, catalytic cracking, treatment of heavy oils, hydrogen balance, environmental concerns, new fuels. Examples of basic, intermediate and end products from petrochemistry. Natural gas and LPG as feedstock, synthesis gas production, preparation and use of hydrogen, methanol synthesis, Fischer–Tropsch, ammonia synthesis. Production of light olefins by steam cracking, dehydrogenation and other routes, use of light olefins.

Teaching:
The course is given as a combination of lectures, exercises, self-study and project work including student presentations.

Course material:
J. Moulijn, M. Makkee and A. van Diepen: Chemical Process Technology
Wiley & Sons, 2001 and articles and handouts.

Exam: Written

TKP4155 Reaction Kinetics and Catalysis

Responsible:
Professor Magnus Rønning

Lecturers:
Professor Magnus Rønning and Adj. Professor Erling Rytter.

Semester: Fall

Level: 4th year

Credits: 7.5 SP

Restricted Admission: No

Course Plan:
Lectures (4 h/week), exercises (2 h/week), self study (6 h/week)

Objectives:
Introduction to important principles and methods of heterogeneous and homogeneous catalysis.

Prerequisites:
Course TKP4110 Chemical Reaction Engineering or similar knowledge.

Contents:
The importance of catalysis as a key technology in chemical and petrochemical industry, in energy production and for the protection of the environment. Definition of catalysis, elementary reactions, chain reactions and catalytic sequences. Kinetic modeling. Catalyst preparation and characterization. Adsorption, desorption, surface area and porosity. Modern theories for surfaces and surface reactions. Internal and external mass and heat transfer in catalyst particles. The effect of diffusion on reaction kinetics. Multifunctional catalysis. Catalysis by transition metal complexes. Ziegler-Natta and single-site polymerisation catalysts.

Teaching form:
The course is given as a combination of lectures, exercises and self-study.

Course material:
Compendium and articles. Information given at semester start.

Exam: Written

TKP4700 Catalysis and petrochemistry

Coordinator for specialization in catalysis and petrochemistry:
Professor Anders Holmen

Course description:
The specialization involves the following modules:

Catalysis and petrochemistry laboratory work/project	15 SP
TKP1 Environmental catalysis	3.75 SP
TKP2 Modeling of catalytic reactions	3.75 SP
TKP3 Heterogeneous catalysis. Advanced course	3.75 SP

2 modules must be chosen, other modules are also electable. The modules give an overall description of the field catalysis and petrochemistry. However, the modules may also be combined with modules from other specializations such as polymer chemistry and reactor technology. Catalysis and petrochemistry laboratory work/project is compulsory for this specialization.

TKP1 Environmental and energy catalysis

Responsible:
Assoc. Professor Hilde J. Venvik

Credits: 3.75 SP

Prerequisites:
TKP4155 Reaction kinetics and catalysis or equivalent knowledge

Module description:
Catalysis occupies an important position within areas such as environmental technology and energy production. Within environmental technology catalysis has become crucial not only for removing of unwanted components such as NO_X, sulfur etc., but also for the development of selective processes. The course will give the fundamentals for catalytic processes for purification of exhaust gases

(NO_X, CO, unburned hydrocarbons etc). Within energy production the focus is on biofuel production, catalytic combustion, production of H_2 and catalysis/reactor technology related to fuel cells. Catalysis for clean production will also be an important part of the course

Teaching methods:
Seminars, self study, exercises/project work with presentations.

Course material:
Articles and excerpts from textbooks.

Language:
English

TKP2 Modeling of catalytic reactions

Responsible:
Professor De Chen

Credits: 3.75 SP

Prerequisites:
TKP 4110 Reaction kinetics and catalysis or equivalent knowledge

Module description:
Microkinetic modeling, catalyst design, elementary reaction steps, theoretical estimation of rate constants, collision and transition state theory, BOC (bond-order conservation) theory, diffusion and reaction in porous catalyst, kinetics for coke formation and deactivation, percolation theory and Monte Carlo simulation, introduction to MATLAB.

Teaching form:
Seminars, self-study, exercises/project work with presentation.

Course material:
Articles and excerpts from textbooks.

Language:
English

TKP3 Heterogeneous catalysis, advanced course

Responsible:
Professor Edd Anders Blekkan

Credits: 3.75 SP

Prerequisites:
TKP4155 Reaction kinetics and catalysis or similar knowledge.

Module description:
The module covers selected topics in heterogeneous catalysis: Characterization and surface area measurements of porous materials and heterogeneous catalysts, deactivation, activity measurements, kinetics and transient kinetic methods, catalytic materials such as metals, supported metals, oxides, zeolites and solid acids.

Teaching methods:
Seminars, self study, exercises/project work with presentations.

Course material:
Articles and excerpts from textbooks.

Language:
English

KP8111 Catalytic conversion of hydrocarbons

Responsible:
Professor Edd Anders Blekkan

Credits: 6 SP

Prerequisites:
TKP4155 Reaction kinetics and catalysis and TKP4150 Petrochemistry and oil refining.

Course description:
The course is given for the last time in spring term 2009.
The emphasis of the course is on reaction mechanisms and kinetics of the catalytic conversion of hydrocarbons. Both homogeneous and heterogeneous reactions are considered, and homogeneous catalytic complexes are discussed as well as surfaces and structures of heterogeneous catalysts. Theories of forming and breaking C-C bonds in hydrocarbons, as well as the influence of simple

reagents like hydrogen, oxygen, water, ammonia and carbon monoxide are reviewed. Examples are chosen from oil refining and petrochemical processes.

Teaching methods:
Seminars, self studies.

Course material:
B.C. Gates: Catalytic Chemistry, J. Wiley and sons, New York 1992, and articles and handouts.

KP8112 Applied heterogeneous catalysis

Responsible:
Professor De Chen

Credits: 6 SP

Prerequisites:
TKP4155 Reaction kinetics and catalysis.

Course description:
The course is given every second year, next time in the fall term 2011.
The course gives an introduction to modern theories for the most important groups of heterogeneous catalysts: Metals, metal oxides and zeolites. Examples of industrial applications are included. An overview of the principles for design and preparation of heterogeneous catalysis will be given. The course includes a kinetic description of the different processes involved in a catalytic cycle: Adsorption, surface reaction and desorption in addition to mass and heat transfer. An introduction to different experimental methods for studying catalytic reactions will also be given.

Teaching methods:
Seminars.

Course material:
Selected articles and handouts.

KP8109 Environmental catalysis.

Responsible:
Professor De Chen

Credits: 6 SP

Course description:
The course is given every second year, next time in spring term 2012.
The course gives an overview on processes and developments in environmental catalysis. It covers catalysis for end of pipe treatments as well as the transition to more environmental processes with no or only limited formation of unwanted byproducts. Catalysis in energy technology (hydrogen as an energy carrier, fuel cells) will be discussed. The design of processes, catalysts and reactors for removal of pollutants is treated. Focus will be on reaction mechanisms and kinetics for the catalytic conversion of pollutants.

Teaching methods:
Seminars.

Course material:
Selected scientific papers.

KP8113 Characterization of heterogeneous catalysts

Responsible:
Professor Magnus Rønning

Credits: 6 SP

Course description:
The course is given every second year, next time in fall term 2010.
In heterogeneous catalysis the reactions take place on the surface of solid materials such as metals, metal oxides and zeolites. It is the conditions on the surface that determines the activity, selectivity and lifetime. Methods for characterization of solid surfaces and of adsorbed components are therefore very important for the understanding of catalytic reactions. The course will give an overview of different methods and a detailed introduction to the use of these methods on catalytic systems. The course covers chemical as well as spectroscopic methods with emphasize on in situ methods.

Course material:
Selected scientific papers.

Course on HMS (Health, Environment and Safety) and Laboratory work

Responsible:
Ass. Professor Hilde J. Venvik

Credits: The course is obligatory and a part of the TKP specialization in catalysis.

Prerequisites: None

Course description:
The goal is to develop a course in HMS (health, environment and safety) covering the activities of the catalysis group. The course is for 5th year students and new Ph.D. students, and is to be held for one week in the beginning of the autumn semester. The goal of the course is

- to give the same qualitative information to everybody working in our laboratories, and thereby improve the safety in the laboratories.
- to improve the attitude to and knowledge in HMS in working life by more teaching and higher demands for this also durting the studies.
- to improve the students' compentense in using the equipment at hand, and thereby improve the efficiency and the quality of the experimental work.
- to introduce the students to the working environment, and to improve the reliance between all the employees.

Teaching methods:
Seminars

Course material:
Handouts

Publications in 2009

1. Borg, Øyvind; Hammer, Nina; Eri, Sigrid; Lindvåg, Odd Asbjørn; Myrstad, Rune; Blekkan, Edd Anders; Rønning, Magnus; Rytter, Erling; Holmen, Anders. *Fischer-Tropsch synthesis over un-promoted and Re-promoted γ-Al2O3 supported cobalt catalysts with different pore sizes.* Catalysis Today 2009 ;Volum 142.(1-2) s. 70-77
2. den Breejen, Johan P.; Radstake, Paul Bernard; Bezemer, G. Leendert; Bitter, JH; Frøseth, Vidar; Holmen, Anders; de Jong, Krijn. *On the Origin of the Cobalt Particle Size Effects in Fischer-Tropsch Catalysis.* Journal of the American Chemical Society 2009 ;Volum 131.(20) s. 7197-7203
3. Chytil, Svatopluk; Glomm, Wilhelm; Blekkan, Edd Anders. *Characterization of Pt/SBA-15 pepared by the deposition-precipitation method.* Catalysis Today 2009 ;Volum 147. s. 217-223
4. Enger, Bjørn Christian; Lødeng, Rune; Holmen, Anders. *Evaluation of reactor and catalyst performance in methane partial oxidation over modified nickel catalysts.* Applied Catalysis A : General 2009 ;Volum 364.(1-2) s. 15-26
5. Enger, Bjørn Christian; Lødeng, Rune; Holmen, Anders. *Modified cobalt catalysts in the partial oxidation of methane at moderate temperatures.* Journal of Catalysis 2009 ;Volum 262. s. 188-198
6. He, Li; Berntsen, H; Ochoa-Fernandez, Esther; Walmsley, John C; Blekkan, Edd Anders; Chen, De. *Co-Ni Catalysts Derived from Hydrotalcite-Like Materials for Hydrogen Production by Ethanol Steam Reforming.* Topics in catalysis 2009 ;Volum 52.(3) s. 206-217
7. Holmen, Anders. *Direct conversion of methane to fuels and chemicals.* Catalysis Today 2009 ;Volum 142. s. 2-8
8. Huang, Fan; Vanhaecke, Estelle Marie M.; Chen, De. *In situ polymerization and characterizations of polyaniline on MWCNT powders and aligned MWCNT films.* Catalysis Today 2009 s. -
9. Kvande, Ingvar; Chen, De; Zhao, Tiejun; Skoe, Inger Marie; Walmsley, John C; Rønning, Magnus. *Hydrogen Oxidation Catalyzed by Pt Supported on Carbon Nanofibers with Different Graphite Sheet Orientations.* Topics in catalysis 2009 ;Volum 52. s. 664-674
10. Li, Ping; Huang, Yi-Li; Chen, De; Zhu, Jun; Zhao, Tiejun; Zhou, Xing-Gui. *CNFs-supported Pt catalyst for hydrogen evolution from decalin.* Catalysis communications 2009 ;Volum 10.(6) s. 815-818
11. Li, Ping; Zhao, Qian; Zhou, Xinggui; Yuan, Weikang; Chen, De. *Enhanced Distribution and Anchorage of Carbon Nanofibers Grown on Structured Carbon Microfibers.* The Journal of Physical Chemistry C 2009 ;Volum 113.(4) s. 1301-1307
12. Lu, Wenxin; Sui, Zhijun; Zhou, Jinghong; Li, Ping; Zhou, Xinggui; Chen, De. *Effect of hydrogen on the synthesis of carbon nanofibers by CO disproportionation on ultrafine Fe3O4.* Asia-Pacific Journal of Chemical Engineering 2009 ;Volum 4.(5) s. 590-595

13. Lögdberg, Sara; Tristantini, Dewi; Borg, Øyvind; Ilver, Lars; Gevert, Börje; Järås, Sven; Blekkan, Edd Anders; Holmen, Anders. *Hydrocarbon production via Fischer-Tropsch synthesis from H2-poor syngas over different Fe-CO/γ-Al2O3 bimetallic catalysts*. Applied Catalysis B: Environmental 2009 ;Volum 89.(1-2) s. 167-182
14. Matam, Santhosh Kumar; Hammer, Nina; Rønning, Magnus; Holmen, Anders; Chen, De; Walmsley, John C; Øye, Gisle. *The nature of active chromium species in Cr-catalysts for dehydrogenation of propane: New insights by a comprehensive spectroscopic study.* Journal of Catalysis 2009 ;Volum 261.(1) s. 116-128
15. Matam, Santhosh Kumar; Chen, De; Holmen, Anders. The influence of pore geometry of Pt containing ZSM-5, Beta and SBA-15 catalysts on dehydrogenation of propane. *Microporous and Mesoporous Materials* 2009 ;Volum 126.(1-2) s. 152-158
16. Matam, Santhosh Kumar; Chen, De; Holmen, Anders; Walmsley, John C. *Dehydrogenation of propane over Pt-SBA-15 and Pt-Sn-SBA-15: Effect of Sn on the disperion of Pt and catalytic behavior*. Catalysis Today 2009 ;Volum 142.(1-2) s. 17-23
17. Mejdell, Astrid Lervik; Jøndahl, Mari; Peters, TA; Bredesen, R; Venvik, Hilde Johnsen. *Effects of CO and CO2 on hydrogen permeation through a similar to 3 mu m Pd/Ag 23 wt.% membrane employed in a microchannel membrane configuration*. Separation and Purification Technology 2009 ;Volum 68.(2) s. 178-184
18. Mejdell, Astrid Lervik; Jøndahl, Mari; Peters, Thijs A.; Bredesen, Rune; Venvik, Hilde Johnsen. *Experimental investigation of a microchannel membrane configuration with a 1.4 μm Pd/Ag23wt% membrane - effects of flow and pressure.* Journal of Membrane Science 2009 ;Volum 327. s. 6-10
19. Mejdell, Astrid Lervik; Peters, Thijs A.; Stange, Marit; Venvik, Hilde Johnsen; Bredesen, Rune. *Performance and application of thin Pd-alloy hydrogen separation membranes in different configurations.* Journal of the Taiwan Institute of Chemical Engineers / Elsevier 2009 ;Volum 40.(3) s. 253-259
20. Myrstad, Rune; Eri, Sigrid; Pfeifer, Peter; Rytter, Erling; Holmen, Anders. *Fischer-Tropsch synthesis in a microstructured reactor.* Catalysis Today 2009;Volum 147. s. S301-S304
21. Ochoa-Fernandez, Esther; Zhao, Tiejun; Rønning, Magnus; Chen, De. *Effects of steam addition on the properties of high temperature ceramic CO2 acceptors.* Journal of environmental engineering 2009 ;Volum 135. s. 397-403
22. Rossetti, I; Fabbrini, L; Ballarini, N; Oliva, C; Cavani, F; Cericola, A; Bonelli, B; Piumetti, M; Garrone, E; Dyrbeck, Hilde; Blekkan, Edd Anders; Forni, L. *V-Al-O catalysts prepared by flame pyrolysis for the oxidative dehydrogenation of propane to propylene.* Catalysis Today 2009 ;Volum 141.(3-4) s. 271-281

23. Sun, Yunfei; Sui, Zhijun; Zhou, Jinhong; Li, Ping; Zhou, Xinggui; Chen, De. *Catalytic decomposition of methane over supported Ni catalysts with different particle sizes.* Asia-Pacific Journal of Chemical Engineering 2009 ;Volum 4.(5) s. 814-820
24. Tucho, Wakshum Mekonnen; Venvik, Hilde Johnsen; Stange, Marit; Walmsley, John C; Holmestad, Randi; Bredesen, Rune. *Effects of thermal activation on hydrogen permeation properties of thin, self-supported Pd/Ag membranes.* Separation and Purification Technology 2009 ;Volum 68.(3) s. 403-410
25. Tucho, Wakshum Mekonnen; Venvik, Hilde Johnsen; Walmsley, John C; Stange, M; Ramachandran, Amutha; Mathiesen, Ragnvald; Borg, Anne; Bredesen, R; Holmestad, Randi. *Microstructural studies of self-supported (1.5-10 mu m) Pd/23 wt% Ag hydrogen separation membranes subjected to different heat treatments.* Journal of Materials Science 2009;Volum 44.(16) s. 4429-4442
26. Zhu, J; Zhou, JH; Zhao, Tiejun; Zhou, XG; Chen, De; Yuan, WK. *Carbon nanofiber-supported palladium nanoparticles as potential recyclable catalysts for the Heck reaction*. Applied Catalysis A : General 2009;Volum 352.(1-2) s. 243-250
27. Zhu, YA; Zhou, XG; Chen, De; Yuan, WK. *Structure-sensitivity of CH3 dissociation on Ni(100) from first-principles calculations*. Asia-Pacific Journal of Chemical Engineering 2009 ;Volum 4.(5) s. 511-517
28. Zhu, Yian; Chen, De; Zhou, Xing-Gui; Yuan, Wei-Kang. *DFT studies of dry reforming of methane on Ni catalyst.* Catalysis Today 2009;Volum 148.(3-4) s. 260-267

Presentations at International and National Meetings 2009

1. Bakhtiary Davvijany, Hamidreza; Hayer, Fatemeh; Phan, Xuyen Kim; Myrstad, Rune; Venvik, Hilde Johnsen; Pfeifer, Peter; Schubert, Klaus; Holmen, Anders. *Experimental study of methanol synthesis in a microchannel reactor.* 21st North American Catalysis Society Meeting; 2009-06-07 - 2009-06-12
2. Bakhtiary, Hamidreza Davijany; Hayer, Fatemeh; Phan, Xuyen Kim; Myrstad, Rune; Pfeifer, Peter; Venvik, Hilde Johnsen; Holmen, Anders. *Methanol synthesis from syngas in amillisecond microstructured reactor.* Norwegian Catalysis Symposium 2009; 2009-11-30 - 2009-12-01
3. Bakhtiary, Hamidreza Davijany; Hayer, Fatemeh; Phan, Xuyen Kim; Myrstad, Rune; Pfeifer, Peter; Venvik, Hilde Johnsen; Holmen, Anders. *Methanol synthesis from syngas in amillisecond microstructured reactor.* Norwegian Catalysis Symposium 2009; 2009-11-30 - 2009-12-01

4. Bergem, Håkon; Otterlei, Camilla; Thorvaldsen, Bodil; Skjølsvik, Per Aksel; Seljestokken, Bente; Rossvoll, Jorunn S.; Blekkan, Edd Anders. *The effect of organic nitrogen compounds on Gas Oil Hydrodesulfurization studied in a pilot plant.* EuropaCat IX; 2009-08-30 - 2009-09-04
5. Bergem, Håkon; Otterlei, Camilla; Thorvaldsen, Bodil; Skjølsvik, Per Aksel; Seljestokken, Bente; Rosvoll, Jorunn S.; Blekkan, Edd Anders. *The effect of organic nitrogen compounds on gas oil hydrodesulfurization studied in a pilot plant.* Norwegian Catalysis Symposium 2009; 2009-11-30 - 2009-12-01
6. Blaylock, D. Wayne; Ogura, Teppei; Dam, Anh Hoang; Wang, Hongmin; Zhu, Yian; Holmen, Anders; Green, William H.; Chen, De. *Computationally-Aided Catalyst Design for Steam Methane Reforming.* 21st North American Catalysis Society Meeting; 2009-06-07 - 2009-06-12
7. Blaylock, D. Wayne; Zhu, Yi-An; Wang, Hongmin; Dam, Anh Hoang; Chen, De; Holmen, Anders; Green, William H. *Steam Methane Reforming Over Ni and Ni/Ag Catalysts - Gaining Mechanistic Insight through DFT and Experiment*. 2009 AIChE Annual Meeting; 2009-11-08 - 2009-11-13
8. Blekkan, Edd Anders. *Biofuels.* NTNU-Tsinghua Symposium; 2009-03-31
9. Blekkan, Edd Anders. *Energy related catalysis research at NTNU*. NTNU-Tsinghua Symposium; 2009-04-01
10. Blekkan, Edd Anders; Holmen, Anders. *Syngas from biomass.* Nordic Climate Cluster workshop; 2009-03-05
11. Boullosa, Eiras Sara; Zhao, Tiejun; Vanhaecke, Estelle Marie M.; Yu, Yingda; Chen, De; Holmen, Anders. *Ce-Zr-Al mixed oxide nanocomposites supported Rh: a promising catalyst for partial oxidation of methane to syngas.* Norwegian catalysis symposium; 2009-11-30 - 2009-12-01
12. Boullosa, Sara Eiras; Zhao, Tiejun; Yu, Yingda; Chen, De; Holmen, Anders. *Alumina-based nanocomposite supported Rh catalysts: an effective and highly stable catalyst for partial oxidation of methane to syngas.* EuropaCat IX : Catalysis for a Sustainable World; 2009-08-30 - 2009-09-04
13. Boullosa, Sara Eiras; Zhao, Tiejun; Yu, Yingda; Chen, De; Holmen, Anders. *Supported Rh on ZrO2-Al2O3 nanocomposite catalyst for catalytic partial oxidation of methane to syngas.* 6th World Congredd on Oxidation Catalysis 6WOOC; 2009-07-05 - 2009-07-10
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15. den Breejen, Johan P.; Radstake, Paul Bernard; Bezemer, G. L.; Frøseth, Vidar; Holmen, Anders; Bitter, Johannes H.; de Jong, Krijn. *On a quantitative description of the cobalt particle size effect in the Fischer-Tropsch reaction.* EuropaCat IX. Catalysis for a Sustainable World; 2009-08-30 - 2009-09-04
16. den Breejen, Johan P.; Radstake, Paul; Bezemer, G. Leendert; Frøseth, Vidar; Holmen, Anders; Bitter, Johannes H.; de Jong, Krijn. *A SSITKA study to understand the cobalt particle size effect in Fischer-Tropsch*

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17. Dam, Anh Hoang; Wang, Hongmin; Dehghan, Roya; Walmsley, John C; Holmen, Anders; Chen, De. *Preparation and characterization of Ni based bimetallic catalysts for steam reforming of methane.* Norwegian Catalysis Symposium 2009; 2009-11-30 - 2009-12-01
18. Dam, Anh Hoang; Wang, Hongmin; Dehghan, Roya; Walmsley, John C; Holmen, Anders; Chen, De. *Preparation and characterization of Ni-Ag surface alloy catalysts.* 21st North American Catalysis Society Conference; 2009-06-07 - 2009-06-12
19. Dar, Hassan Jamil; Nanot, Sandro U.; Jakobsen, Hugo Atle; Tangstad, Elisabeth; Chen, De. *Simulation for Oxidative Dehydrogenation of Ethane to Ethylene.* inGap Summerschool in Heterogeneous Catalysis; 2009-06-21 - 2009-06-26
20. Dehghan, Roya; Walmsley, John C; Hansen, Thomas W.; Wagner, Jakob B.; Holmen, Anders; Rytter, Erling; Borg, Øyvind. *In-situ electron microscopy study of catalyst nano particle reduction.* Norwegian Catalysis Symposium 2009; 2009-11-30 - 2009-12-01
21. Dehghan, Roya; Walmsley, John C; Holmen, Anders; Midgley, Paul A.; Hungria, Ana B.; Hernandez-Garrido, Juan C.; Chen, De. *TEM study of hydrotalcite derived Ni catalysts.* EuropaCat IX : Catalysis for a Sustainable World; 2009-08-30 - 2009-09-04
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23. Dehghan-Niri, Roya; Holmestad, Randi; Walmsley, John C; Holmen, Anders; Rytter, Erling; Hansen, Thomas W.*Advanced TEM study of Co Fischer-Tropsch catalyst*. NanoMat meeting; 2009-06-15 - 2009-06-19
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26. Gorelkin, Ilya; Blekkan, Edd Anders. *Possible reaction mechanisms of the catalytic dehydrogenation of propane.* Norwegian Catalysis Symposium 2009; 2009-11-30 - 2009-12-01
27. Hayer, Fatemeh; Bakhtiary, Hamidreza Davijany; Myrstad, Rune; Venvik, Hilde Johnsen; Holmen, Anders. *Experimental study of compact dimethyl ether synthesis from syngas.* Norwegian Catalysis Symposium 2009; 2009-11-30 - 2009-12-01
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29. Holmen, Anders. *Deactivation of Fischer-Trospch catalysts. 11th International Symposium on Catalyst Deactivation*; 2009-10-25 - 2009-10-28
30. Holmen, Anders. *Fischer-Tropsch synthesis on Co supported on modified aluminas.* University of Wisconsin; 2009-04-21
31. Holmen, Anders. *Fuel production by Fischer-Tropsch synthesis with CO/H2 from fossil and renewable feeds*. University of Minnesota; 2009-04-23
32. Holmen, Anders; Enger, Bjørn Christian; Lødeng, Rune; Boullosa, Eiras Sara; Chen, De. *Partial Oxidation of Methane.* 2009 AIChE Annual Meeting; 2009-11-08 - 2009-11-13
33. Huang, Fan; Vanhaecke, Estelle Marie M.; Chen, De. *In-situ polymerization of a composite PANI/carbon nanostructures*. InGap-Nanocat Summerschool in Heterogeneous catalysis: Nano designed catalysts: from molecules to industrial processes; 2009-06-21 - 2009-06-26
34. Huang, Fan; Vanhaecke, Estelle Marie M.; Rønning, Magnus; Chen, De. *Composite of conducting polymers and carbon nanostructures for energy storage.* Norwegian Catalysis Symposium 2009; 2009-11-30 - 2009-12-01
35. Kazi, Saima Sultana; Vanhaecke, Estelle Marie M.; Zhao, Tiejun; Rønning, Magnus; Chen, De. *Sol-gel derived zirconia coated calcium oxide nanoparticles for CO2-capture.* Norwegian Catalysis Symposium 2009; 2009-11-30 - 2009-12-01
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38. Matam, Santhosh Kumar; Hammer, Nina; Rønning, Magnus; Holmen, Anders; Chen, De; Walmsley, John C; Øye, Gisle. *The nature of active Cr species in Cr-cataysts for dehydrogenation of propane: Neew insights by a comprehensive spectoscopi study.* EuropaCar IX : Catalysis for a Sustainable Wold; 2009-08-30 - 2009-09-04
39. Mejdell, Astrid Lervik; Peters, Thijs A.; Bredesen, Rune; Chen, De; Venvik, Hilde Johnsen. *5-3 µm Pd/23wt.% Ag membranes applied in a microchannel membrane configuration - effects of flow, pressure and competitive adsorption of CO and CO2.* ICOSCAR-3, 3rd International Conference on STRUCTURED CATALYSTS AND REACTORS; 2009-09-27 - 2009-09-30
40. Mihai, Oana; Chen, De; Holmen, Anders. *Comparative study regarding preparation methods of perovskite-type oxides LaFeO3 catalysts for methane partial oxidation.* inGAP-NANOCAT Summer School; 2009-06-21 - 2009-06-26

41. Mihai, Oana; Chen, De; Holmen, Anders. *Synthesis of perovskites using carbon nanotubes as templates and their applications in methane partial oxidation.* Norwegian Catalysis Symposium 2009; 2009-11-30 - 2009-12-01
42. Muthuswamy, Navaneethan; Ochal, Piotr; Gomez, Jose Luis de la Fuente; Tsypkin, Mikhail; Rønning, Magnus; Sunde, Svein; Chen, De. *Electro-oxidation of CO and methanol on Ru-Pt core-shell nanoparticles supported on carbon materials.* Norwegian Catalysis Symposium 2009; 2009-11-30 - 2009-12-01
43. Myrstad, Rune; Eri, Sigrid; Pfeifer, Peter; Rytter, Erling; Holmen, Anders. *Fischer-Tropsch synthesis in a microstructured reactor*. Norwegian Catalysis Symposium 2009; 2009-11-30 - 2009-12-01
44. Noor, Tayyaba; Lind, Anna Maria; Holmen, Anders; Chen, De. *Synthesis and characterization of Ni hydrotelcite catalyst for hydrogen production using co-parcipitation spray drying, microemulsion method.* Norwegian Catalysis Symposium 2009; 2009-11-30 - 2009-12-01
45. Patanou, Eleni; Chen, De; Blekkan, Edd Anders. *Microcalorimetry and mikrokinetic modelling of catalytic reactions.* InGap –Nanocat Summerschool in Heterogeneous catalysis: Nano designed catalysts: from molecules to industrial processes; 2009-06-21 - 2009-06-26
46. Peters, Thijs A.; Stange, Marit; Venvik, Hilde Johnsen; Bredesen, Rune. *Properties and application of supported Pd-23%Ag membranes for H2 production and separation.* Hydrogen and Fuel Cells in the Nordic Countries - 2009; 2009-11-24 - 2009-11-26
47. Phan, Xuyen Kim; Myrstad, Rune; Venvik, Hilde Johnsen; Thormann, Janina; Pfeifer, Peter; Holmen, Anders. *Experimental study of methanol synthesis in a PdCeO2 stacked microchannel reactor.* Norwegian Catalysis Symposium 2009; 2009-11-30 - 2009-12-01
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49. Radstake, Paul Bernard; Håkonsen, Silje Fosse; Rønning, Magnus; Holmen, Anders. *Oxidative Dehydrogenation of Ethane at Short Contact Times.* 3rd International Conference on Structured Catalysts and Reactors; 2009-09-27 - 2009-09-30
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51. Rønning, Magnus. *Catalyst studies at real working conditions.* Seminar at Department of Chemical Engineering, University of Zaragoza; 2009-11-10
52. Rønning, Magnus. *Characterisation of catalysts at their working conditions.* Nanoduramea Summer School - Synthesis and characterisation of carbon supported platinum and platinum alloy catalysts; 2009-06-08 - 2009-06-09

53. Rønning, Magnus. *In situ characterisation techniques for studying catalysts at realistic working conditions.* Norwegian Synchrotron User Meeting; 2009-06-18 - 2009-06-19
54. Rønning, Magnus; Tsakoumis, Nikolaos; Voronov, Alexey; Borg, Øyvind; Rytter, Erling; Holmen, Anders. *Deactivation studies of Co-Re/γ-Al2O3 Fischer-Tropsch catalyst.* EuropaCat IX : Catalysis for a Sustainable World; 2009-08-30 - 2009-09-04
55. Rønning, Magnus; Voronov, Alexey Sergeevich; Tsakoumis, Nikolaos; Borg, Øyvind; Hammer, Nina; Rytter, Erling; Holmen, Anders. *Complimentary in situ characterisation techniques at realistic working conditions for the Fischer-Tropsch synthesis.* 14th International Conference on X-ray Absorption Fine Structure; 2009-07-26 - 2009-07-31
56. Rønning, Magnus; Voronov, Alexey Sergeevich; Tsakoumis, Nikolaos; Borg, Øyvind; Rytter, Erling; Holmen, Anders. *Decoupling of the deactivation mechanisms in Co-based Fischer-Tropsch catalysts by a wide range of in situ spectroscopies at realistic working conditions.* Operando_III, Third International Congress on Operando Spectroscopy; 2009-04-19 - 2009-04-23
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58. Tsakoumis, Nikolaos; Voronov, Alexey Sergeevich; Borg, Øyvind; Rønning, Magnus; Rytter, Erling; Holmen, Anders. *Deactivation studies on Re promoted Co/γ-Al2O3 catalysts for Fischer-Tropsch synthesis.* 11th International Symposium on Catalyst Deactivation; 2009-10-25 - 2009-10-28
59. Tsakoumis, Nikolaos; Voronov, Alexey Sergeevich; Rønning, Magnus; Borg, Øyvind; Rytter, Erling; Holmen, Anders. *Insights into catalyst deactivation phenomena in Co-based Fischer-Tropsch.* Norwegian Catalysis Symposium 2009; 2009-11-30 - 2009-12-01
60. Vanhaecke, Estelle Marie M.; Huang, Fan; Chen, De; Rønning, Magnus. *Aligned carbon nanotubes array, synthesis and applications in composite design for new energy and energy storage.* EuroNanoForum; 2009-06-02 - 2009-06-05
61. Vanhaecke, Estelle Marie M.; Huang, Fan; Chen, De; Rønning, Magnus. *Carbon nanostructures synthesis on foils.* Norwegian Catalysis Symposium 2009; 2009-11-30 - 2009-12-01
62. Vanhaecke, Estelle Marie M.; Huang, Fan; Chen, De; Rønning, Magnus. *Carbon nanotubes Synthesis Composite on Foils.* Shinschu University seminar; 2009-03-12
63. Vanhaecke, Estelle Marie M.; Huang, Fan; Chen, De; Rønning, Magnus. *Carbon nanotubes Synthesis Composite on Foils.* Shinschu University seminar; 2009-03-12

64. Voronov, Alexey Sergeevich; Tsakoumis, Nikolaos; Borg, Øyvind; Rytter, Erling; Holmen, Anders; Rønning, Magnus. *Deactivation studies in Co-based Fischer-Tropsch catalysts.* Norwegian Symposium on catalysis; 2009-11-30 - 2009-12-01
65. Voronov, Alexey Sergeevich; Tsakoumis, Nikolaos; Borg, Øyvind; Rytter, Erling; Holmen, Anders; Rønning, Magnus. *Deactivation studies of Co-based Fischer-Tropsch catalysts by in situ spectroscopies at realistic working conditions.* 11th International Symposium on Catalyst Deactivation; 2009-10-25 - 2009-10-28
66. Wangen, Espen Standal; Malik, Azhar; Pagels, Joakim; Lindskog, Magnus; Sanati, Mehri; Blekkan, Edd Anders. *On the steam reforming of producer gas for the production of clean bio-syngas.* Norwegian Symposium on Catalysis; 2009-11-30
67. Wangen, Espen Standal; Trehjørningen, Kristin Rem; He, Li; Chen, De; Blekkan, Edd Anders. *Reforming raw synthesis gas from wood gasification.* 21st North American Catalysis Society Meeting; 2009-06-07 - 2009-06-12
68. Zhao, Tiejun; Boullosa, Eiras Sara; Yu, Yingda; Yu, Xiaofeng; Raaen, Steinar; Rønning, Magnus; Chen, De; Holmen, Anders. *Synthesis and catalytic performance of high-temperature stable nanocomposites by a versatile nanoparticle-mediated Pechini method.* Europcat IX; 2009-08-30 - 2009-09-04
69. Zhao, Tiejun; Yu, Yingda; Chen, De; Rønning, Magnus. *Carbon nanofiber/carbon felt supported Cu-CeO2 catalyst: a promising structured catalyst for preferantial oxidation of CO in H2-rich gases.* Norwegian Catalysis Symposium 2009; 2009-11-30 - 2009-12-01
70. Zhao, Tiejun; Yu, Yingda; Yu, Xiaofeng; Raaen, Steinar; Chen, De; Rønning, Magnus. *Preferential oxidation of CO in H2-rich gases over the Pechini-method- derived Cu-CeO2 nanocomposite and monolith catalysts.* China-North America Workshop on Fuel Cell Science and Technology; 2009-08-13 - 2009-08-15
71. Zhu, Jun; Rønning, Magnus; Holmen, Anders. *Platinum nanoparticle shape effect on propane dehydrogenation.* Norwegian Catalysis Symposium 2009; 2009-11-30 - 2009-12-01
72. Rane, Shreyas Pandurang; Borg, Øyvind; Rytter, Erling; Holmen, Anders. *Effect on cobalt particle size, alumina and its porosity on hydrocarbon selectivity in Fischer-Tropsch synthesis.* Norwegian Catalysis Symposium 2009; 2009-11-30 - 2009-12-01
73. Rane, Shreyas Pandurang; Tveten, Erik Zakarias; Borg, Øyvind; Rytter, Erling; Holmen, Anders. *Performance of supported Co catalysts fro Fischer-Tropsch synthesis.* 21st North American Catalysis Society Meeting; 2009-06-07 - 2009-06-12
74. Wang, Hongmin; Dam, Anh Hoang; Blaylock, Wayne; Ggura, Tappei; Zhu, Yian; Holmen, Anders; Greeen, William H.. *Kinetic study of methane steam reforming over hydrotalcite-based Ni catalyst modified by different metals.* Norwegian Catalysis Symposium 2009; 2009-11-30 - 2009-12-01

75. Wang, Hongmin; Holmen, Anders; Chen, De.
Optimum design and operation of a hydrogen generation by natural gas autothermal reforming system. 1st Trondheim Gas Technology Conference; 2009-10-21 - 2009-10-22
76. Yang, Jia; Tveten, Erik Zakarias; Borg, Øyvind; Rytter, Erling; Holmen, Anders. *Effect of Support on the Intrinsic Activity and Selectivity for Co-based Fischer-Tropsch Catalysts.* EuropaCat IX : Catalysis for a Sustainable World; 2009-08-30 - 2009-09-04
77. Vanhaecke, Estelle Marie M.; Chen, De; Huang, Fan.
Nanostructured materials based on carbon nanostructures: candidate for solar cells. Oppdal Workshop on PV Materials; 2009-03-19 - 2009-03-21

Seminar on Catalysis in Methane Activation
Tuesday, January 13 2009, Aud. PFI 5101, NTNU.

Session 1
Chairman: Prof. De Chen

10:00-10:10 Welcome address
Prof. De Chen

10:10-10:40 Hydrogen production with CO_2 capture
Dr. J. Bragdø Smith, StatoilHydro

10:40-11:10 Hydrogen Production via Steam Methane Reforming: *From Atoms to Process*
Prof. William. H. Green, MIT

11:10-11:40 Steam Methane Reforming Microkinetics over Ni and Ni/Ag Catalysts
Dr. Wayne Blaylock, MIT

Lunch

Session 2
Chairman: Prof. Anders Holmen

13:00-13:25 DFT investigation of carbon dissolution and diffusion in Ni based catalysts
Dr. Yi-An Zhu, East China University of Science and Technology

13:25-13:50 Synthesis and characterization of Ni based catalysts
Hong Anh Dam, NTNU

13:50-14:15 Kinetic study of steam methane reforming on Ni based catalysts,
Dr. Hongmin Wang, NTNU

14:15-14:30 Coffee

14:30-14:55 Nanocomposites for syngas production by methane partial oxidation
Sara Boullosa Eiras, NTNU

14:55-15:20 Nanomaterials for syngas production from chemical looping methane partial oxidation
Oana Mihai, NTNU

15:20-15:40 Catalysis in methane activation: Closing remarks
Prof. De Chen, NTNU

KINCAT Guest lecture

Dr. ing. Peter Pfeifer, Karlsruhe Institute of Technology:

"Considerations of mass and heat transfer for scale-up of microreactors"

Wednesday 4th of November at 14:15 in auditorium R9.

The lecture lasts about 2x45 mins. and is open to everyone.

Abstract:

Microchannel or microstructured reactors are commonly discussed as perfect tools for kinetic measurements and that they would enable easy process intensification and scale-up due to enhanced heat and mass transfer. The assumption that there is direct access in microreactors to intrinsic kinetics, however, has to be proven by suitable methods and derived equations for fixed bed reactors are seldom valid. Moreover, a simple scale-up by multiplying channels is often accompanied with questions of equal flow distribution and distribution of heat inside larger multi-channel arrangements. The talk will give information about analysis methods and scale-up strategies, which are currently discussed.

Peter Pfeifer is since 2000 Group Leader of “Chemical Micro Process Engineering” at Institute of Micro Process Engineering, Karlsruhe Institute of Technology (KIT), formerly Forschungszentrum Karlsruhe (FZK). He has Diploma (MSc) in Chemical Engineering from the University of Erlangen in 1997, and obtained his Dr.-Ing. (PhD) in Chemical Engineering from the University of Erlangen in 2003, thesis entitled "Methanol-Steam Reforming in Microstructured Reactors for Hydrogen Generation in Fuel Cell Driven Cars". Since 2008 he is also lecturer at Faculty of Chemical Engineering, University of Karlsruhe. Pfeifer is co-author of more than 50 scientific papers, patents and book chapters on microstructured reactors.

SFFE & GTS Lunch Colloquium:
Tuesday December 8th,
12:00-13:00
Auditorium S1, Sentralbygget

Førsteamanuensis Hilde Venvik, NTNU

Biofuels –

Catalytic conversion of biomass to liquid fuels

Find out why catalysts are important in efficient conversion of biomass to liquid fuels, and hear about the most recent breakthroughs in this area.

Please register at www.ntnu.no/gass/seminars by Monday 7/12 at 09:00 to receive a free lunch. The seminar is open for students and researchers at NTNU and SINTEF.

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More information at **www.sffe.no** and **www.ntnu.no/gass**

Norwegian Catalysis Symposium 2009
Programme

Auditorium R8, Realfagbygget (Science building), Høgskoleringen 5, Gløshaugen, Trondheim.

Monday November 30, 2009

09:00 Coffe

09:50 Welcome
Anders Holmen

10:00 -12:00 Session 1. Chair: **Erling Rytter, Hilde Venvik**.

10:00 - 10:20 *On the steam reforming of producer gas for the production of clean bio-syngas.*
Espen Standal Wangen, Azhar Malik, Mehri Sanati, Edd A. Blekkan. Dept. Chemical Engineering, NTNU, Trondheim, Norway/Lund University, Ergonomics and Aerosol Technology Design Sciences, Lund, Sweden.

10:20 - 10:40 *The influence of additives in defining the active phase of the ethylene oxychlorination catalyst.*
Naresh Babu Muddada, U. Olsbye, L. Caccialupi, F. Cavani, T. Fuglerud, A. Marsella, S. Vidotto, G. Leofanti, D. Gianolio, S. Bordiga, C. Lamberti. inGAP, Department of Chemistry, University of Oslo, Norway/Dipartimento di Chimica Industriale e dei Materiali, Università di Bologna, Bologna, Italy/INEOS Norge A/S, Porsgrunn, Norway/INEOS Technologies - Vinyls R&D, Porto Marghera (Venezia), Italy/Consultant, Canegrate (Milano), Italy/ Department of Inorganic, Physical and Materials Chemistry and NIS centre of excellence, University of Torino, Italy.

10:40 -11:00 *Platinum nanoparticle shape effect on propane dehydrogenation*.
Jun Zhu, Magnus Rønning, Yingda Yu, Anders Holmen, De Chen. Dept. of Chemical Engineering/Dept. of Materials Technology, NTNU, Trondheim, Norway.

11:00 - 11:20 *Conversion of methanol to hydrocarbons over 10-ring uni-directional acidic H-ZSM-22.*
Shewangizaw Teketel, Stian Svelle, Karl-Petter Lillerud, Pablo Beato, Unni Olsbye. inGAP, Dept. of Chemistry, University of Oslo, Norway/Haldor Topsøe, Lyngby, Denmark.

11:20 - 11:40 *Fischer-Tropsch synthesis in a microstructured reactor.*
Rune Myrstad, Sigrid Eri, Peter Pfeifer, Erling Rytter, Anders Holmen. SINTEF Materials and Chemistry, Trondheim, Norway/Statoil, Research Centre, Trondheim, Norway/ Forschungzentrum Karlsruhe, Eggenstein-Leopoldshafen, Germany/NTNU, Trondheim, Norway.

11:40 - 12:00 *Experimental study of compact dimethyl ether synthesis from syngas.*
Fatemeh Hayer, Hamidreza Bakhtiary D., Rune Myrstad, Hilde J. Venvik, Anders Holmen. Dept. of Chemical Engineering, NTNU,Trondheim, Norway/SINTEF Materials and Chemistry, Trondheim, Norway.

12:00 Lunch

13:00 - 16:00 Session 2. Chair: Unni Olsbye, Edd A. Blekkan.

13:00 Plenary I: *Mass spectrometry for the analysis of zeolite formation processes.* Professor Ferdi Schüth, Max-Planck Institute, Mülheim, Germany

14:00 - 14:20 *Effect of support on the intrinsic activity and selectivity for Co-based Fischer-Tropsch catalysts*.
Jia Yang, Erik Tveten, Øyvind Borg, Erling Rytter, Anders Holmen. Dept. of Chemical Engineering, NTNU, Trondheim, Norway/Statoil Research Centre, Trondheim, Norway.

14.20 - 14:40 *Deactivation studies in Co-based Fischer-Tropsch catalysts.*
Alexey Voronov, Nikolaos E. Tsakoumis, Øyvind Borg, Erling Rytter, Anders Holmen, Magnus Rønning. Dept. of Chemical Engineering, NTNU, Trondheim, Norway/Statoil Research Centre, Trondheim, Norway.

14:40 - 15:00 *In-situ electron microscopy study of catalyst nano particle reduction.*
Roya Dehghan, John C. Walmsley, Thomas W. Hansen, Jakob B. Wagner, Anders Holmen, Erling Rytter, Øyvind Borg. Dept of Physics, NTNU, Trondheim, Norway/SINTEF Materials and Chemistry,Trondheim, Norway/Electron Nanoscopy Centre for Technical University of Denmark/Dept. of Chemical Engineering, NTNU, Trondheim, Norway/Statoil R&D Research Centre, Trondheim, Norway.

15:00 - 15:20 *Performance of rare-earth metal bis(tetramethylaluminate) complexes in isoprene polymerization: Ancillary ligand, cocatalyst, and metal size effects.*
Rannveig Litlabø, Melanie Zimmermann, H. Martin Dietrich, Karl W. Törnroos and Reiner Anwander. Dept of Chemistry, University of Bergen, Norway/Institutt für Anorganische Chemie, Universität Tübingen, Germany.

15:20 - 15:40 *Mechanistic analysis and catalytic improvement of a highly cis-selective Rh(I) cyclopropanation catalyst.*
Marianne Lenes Rosenberg, Mats Tilset, Dept. of Chemistry, University of Oslo, Norway.

15:40 -16:00 *The mechanism of phosphine dissociation in Grubbs catalysts for olefin metathesis.*
Yury Minenkov, G. Occhipinti and Vidar R. Jensen, Dept. of Chemistry, University of Bergen, Norway.

16:00 - 16:30 Annual Meeting Catalysis Group, Norwegian Chemical Society. Stian Svelle, University of Oslo, President.

16:30 – 18:00 Poster presentations

20:45 Dinner at Lian Restaurant (transport from the city centre at 20:00).

Tuesday December 1, 2009

09:00 - 12:00 Session 3 Chair: Steinar Kvisle, Magnus Rønning.

09:00 Plenary II. *Selective nanocatalysis of organic transformation by metals. Concepts, instruments and model systems.* Professor Gabor Somorjai, University of California, Berkeley, USA

10:00 - 10:20 *Utilization of CO_2 via Catalysis with Ionic Liquids.*

Richard H. Heyn, Terje Didriksen, Silje Håkonsen, Knut Thorshaug and Ørnulv B. Vistad. SINTEF Materials and Chemistry, Dept. of Process Chemistry, Oslo, Norway

10:20 - 10:40 *Implementation of parallel/high throughput strategies for evaluation of deNOx catalyst systems.*
Lenka Hannevold, Duncan Akporiaye, Arne Karlsson, Martin Plassen, Elisabeth Myhrvold. Joanna Prostak. SINTEF, Material and Chemistry, Oslo, Norway.

10:40 - 11:00 *The effect of organic nitrogen compounds on gas oil hydrodesulfurization studied in a pilot plant.*
Håkon Bergem, Camilla Otterlei, Bodil Thorvaldsen, Per Aksel Skjølsvik, Bente Seljestokken, Jorunn S. Rosvoll, Edd A. Blekkan. Dept. of Process Technology, SINTEF, Trondheim, Norway/Dept. of Chemical Engineering, NTNU, Trondheim, Norway/Statoil Research Centre, Trondheim, Norway.

11:00 - 11:20 *Functionalized zirconium-MOFs: Stability and applications*.
Merete Hellner Nilsen, Søren Jakobsen, Mathivathani Kandiah, Fredrik Lundvall, Sandrine Bénard, Sandro N. Usseglio, Unni Olsbye, Mats Tilset, Karl Petter Lillerud
inGap, Dept. of Chemistry, University of Oslo, Norway.

11:20 - 11:40 *Sol-gel derived zirconia coated calcium oxide nanoparticles for CO_2 capture.*
Kazi Saima Sultana, Estelle Vanhaecke, Tiejun Zhao, Magnus Rønning and De Chen.
Dept. of Chemical Engineering, NTNU, Trondheim, Norway.

11:40 - 12:00 *Formation of mesoporosity in zeolite H-SSZ-13 by desilication*
Linn Sommer, Davide Mores, Stian Svelle, Michael Stöcker, Bert Weckhuysen, Unni Olsbye. Center for Materials Science and Nanotechnology/inGAP, Dept. of Chemistry, University of Oslo, Norway/Inorganic Chemistry and Catalysis, DEBYE Institute for Nanomaterials Science, Utrecht University, Utrecht, The Netherlands/SINTEF Materials and Chemistry, Dept. of Hydrocarbon Process Chemistry, Oslo, Norway.

12:00 - 12:15. *The KOSK-II Programme*. Mats Tilset, University of Oslo, Chair of the KOSK Programme Board.

12:15 Lunch

13:00 - Annual meeting inGAP - Closed meeting (Organizer: Unni Olsbye, Univ. of Oslo)

13:00 - Laboratory tour (Organizer: Karin W. Dragsten, NTNU)

Poster presentations

P1
Spray drying of porous alumina support for Fischer-Tropsch catalysis.
Anna Lind, Anders Holmen, Sigrid Eri, Torild Hulsund Skagseth, Erling Rytter. SINTEF Materials and Chemistry,Trondheim, Norway/Dept. of Chemical Engineering, NTNU, Trondheim, Norway/Statoil Research Centre, Trondheim, Norway.

P2
Electro-oxidation of CO and methanol on Ru-Pt core-shell nanoparticles supported on carbon materials.
Navaneethan Muthuswamy, M. Piotr Ochal, Jose Gomez, Mikhail Tsypkin, Magnus Rønning, Svein Sunde, De Chen. Dept. of Chemical Engineering /Dept. of Material Science and Engineering, NTNU, Trondheim, Norway.

P3
Possible reaction mechanisms of the catalytic dehydrogenation of propane.
Ilya V. Gorelkin, Edd A. Blekkan. Dept. of Chemical Engineering, NTNU, Trondheim, Norway.

P4
Preparation and characterization of Ni based bimetallic catalysts for steam reforming of methane.
Anh H. Dam, H. M. Wang, Roya Dehghan, John Walmsley, Anders Holmen and De Chen Dept. of Chemical Engineering/Dept. of Physics, NTNU, Trondheim, Norway

P5
In situ diffuse reflectance FTIR (DRIFT) spectroscopy on supported nickel and noble metal catalysts.
Christoph Sprung, B. Arstad, U. Olsbye. Dept. of Chemistry, Center of Materials Science and Nanotechnology, University of Oslo, Norway/SINTEF Materials and Chemistry, Oslo, Norway.

P6
Alkylaluminate chemistry of alkaline-earth metals and divalent lanthanides.
Olaf Michel, Christian Meermann, Karl W. Törnroos, Reiner Anwander.
Dep. of Chemistry, University of Bergen, Norway/Institutt für Anorganische Chemie, Universität Tübingen, Germany.

P7
CHA and SAPO-34: Lattice stability dependence on position of acid sites.
Mahsa Zokaie, Ole Swang, Stian Svelle, Merete Hellner Nilsen, Unni Olsbye and Karl Peter Lillerud. inGAP Centre for Research-Based Innovation/Center for Materials Science and Nanotechnology, Dept. of Chemistry, University of Oslo,Norway.

P8
Development of Au catalysts for the functionalization of alkanes: Precursor synthesis and C-H activation.
Ajay Venugopal, Manik Kumer Ghosh, Richard H.Heyn, Anthony P. Shaw, Ole Swang, Karl W. Törnroos and Mats Tilset. SINTEF Materials and Chemistry, Dept. of Process Chemistry, Oslo, Norway/Dept. of Chemistry, University of Bergen, Norway/Center of Theoretical and Computational Chemistry, Dept. of Chemistry, University of Oslo, Norway.

P9
Investigations into structure-reactivity relationships in rare-earth metal-promoted Ziegler-Natta polymerization.
H. Martin Dietrich, Karl W.Törnroos and Reiner Anwander. Dept. of Chemistry, University of Bergen, Norway/Institut für Anorganische Chemie, Universität Tübingen, Tübingen, Germany.

P10
Microstructural observations in metal dusting studies.
John C. Walmsley, J.Z. Albertsen and J. Friis. SINTEF Materials and Chemistry, Trondheim, Norway/Dept. of Materials Science and Engineering, NTNU.Trondheim, Norway/Statoil, Research Centre, Trondheim, Norway.

P11
Methanol synthesis from syngas in a millisecond microstructured reactor.
Hadimreza Bakhtiary, Fatemeth Hayer, Xuyen Kim Phan, Rune Myrstad, Peter Pfeifer, Hilde J. Venvik, Anders Holmen. Dept. of Chemical Engineering, NTNU, Trondheim, Norway/ SINTEF Materials and Chemistry, Trondheim, Norway/Karlsruhe Institute of Technology, Institute for Micro Process Engineering, Eggenstein-Leopoldshafen, Germany.

P12
Experimental study of methanol synthesis in a $PdCeO_2$ stacked microchannel reactor.
Xuyen Kim Phan, Hamidreza Bakhtiary, Rune Myrstad, Hilde J. Venvik, Janina Thormann, Peter Pfeifer, Anders Holmen. Dept. of Chemical Engineering, NTNU, Trondheim, Norway/SINTEF Materials and Chemistry, Trondheim, Norway/Karlsruhe Institute of Technology, Institute for Micro Process Engineering, Eggenstein-Leopoldshafen, Germany.

P13
Synthesis and characterization of Ni hydrotelcite catalyst for hydrogen production using co-precipitation, spray drying, microemulsion method.
Tayyaba Noor, Anna Lind, Anders Holmen, De Chen. Dept. of Chemical Engineering, NTNU, Trondheim, Norway/SINTEF Materials and Chemistry, Trondheim, Norway.

P14
Kinetic study of methane steam reforming over hydrotalcite-based Ni catalyst modified by different metals.
Hongmin Wang, Ahn H. Dam, D. Wayne Blaylock, Tappei Ogura, Yian Zhu, Anders Holmen, Willian H. Green, De Chen. Massachusetts Institute of Technology, Cambridge, Massachusetts, USA/Dept of Chemical Engineering, NTNU, Trondheim, Norway.

P15
Ce-Zr-Al mixed oxide nanocomposites supported Rh: a promising catalyst for partial oxidation of methane to syngas.
Sara Boullosa-Eiras, Tiejun Zhao, Estelle Vanhaecke, Yingda Yu, De Chen, Anders Holmen Dept. of Chemical Engineering/Dept. of Material Science and Technology, NTNU, Trondheim, Norway.

P16
Microcalorimetry and microkinetic modelling of catalytic reactions.
Eleni Patanou, De Chen, Edd A. Blekkan. Dept. of Chemical Engineering, NTNU, Trondheim, Norway.

P17
Insights into catalyst deactivation phenomena in Co-based Fischer-Tropsch.
Nikolaos E. Tsakoumis, Alexey Voronov, Magnus Rønning, Øyvind Borg, Erling Rytter and Anders Holmen. Dept. of Chemical Engineering, NTNU, Trondheim, Norway/Statoil R&D, Research Centre, Trondheim, Norway.

P18
Effect on cobalt particle size, alumina and its porosity on hydrocarbon selectivity in Fischer-Tropsch synthesis.
Shreyas Rane, Øyvind Borg, Erling Rytter, Anders Holmen.Dept. of Chemical Engineering, NTNU, Trondheim, Norway/Statoil, Reseach Center, Trondheim, Norway.

P19
Composite of conducting polymers and carbon nanostructures for energy storage.
Fan Huang, Estelle Vanhaecke, Magnus Rønning, De Chen. Dept. of Chemical Engineering, NTNU, Trondheim, Norway.

P20
Elaboration of model compounds for catalysis by the means of ALD.
Madeleine Diskus, Ola Nilsen and Helmer Fjellvåg.
inGAP Centre for Research-Based Innovation/Center for Materials Science and Nanotechnology, Dept. of Chemistry, University of Oslo, Norway.

P21
Synthesis of perovskites using carbon nanotubes as templates and their applications in methane partial oxidation.
Oana Mihai, De Chen, Anders Holmen. Dept. of Chemical Engineering, NTNU, Trondheim, Norway.

P22
Carbon nanostructures synthesis on foils.
Estelle Vanhaecke, Fan Huang, De Chen, Magnus Rønning. Dept. of Chemical Engineering, NTNU, Trondheim, Norway.

P23
Amino-functionalized Zr-MOF as catalyst for the Knoevenagel reaction
Sandrine Bénard, Søren Jakobsen, Mathivathani Kandiah, Merete Hellner Nilsen, Fredrik Lundvall, Sandro N. Usseglio, Unni Olsbye, Mats Tilset, Karl Petter Lillerud.
inGAP Centre for Research-Based Innovation, Dept. of Chemistry, University of Oslo, Norway.

P24
The polar functional group tolerance of transition metal catalysts for olefin polymerization
Wouter Heyndrickx, G. Occhipinti and Vidar R. Jensen. Dept. of Chemistry, University of Bergen, Norway.

P25
Catalysts for sorbent enhanced steam reforming (SER) of methane in temperature swing reactors.
Christoph Sprung, Bjørnar Arstad, Unni Olsbye. Dept. of Chemistry, Center of Materials Science and Nanotechnology, University of Oslo, Norway/SINTEF Materials and Chemistry, Oslo, Norway.

P26

Carbon nanofiber/carbon felt supported Cu-CeO_2 catalyst: a promising structured catalyst for preferential oxidation of CO in H_2- rich gases.

Tiejun Zhao, Yingda Yu, De Chen, Magnus Rønning. Dept. of Chemical Engineering/Dept. of Material Science and Technology, NTNU, Trondheim, Norway.