Annual Report

2011

Catalysis Group – SINTEF – NTNU

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 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:

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Annual Report 2011
KINCAT
Strong Point Centre Kinetics and Catalysis

Contents

KinCat Members
Department of Chemical Engineering
Catalysis Group

Academic staff:
Professor Edd A. Blekkan
Professor De Chen
Professor Anders Holmen
Professor Magnus Rønning
Professor Hilde J. Venvik
Adjunct Professor Erling Rytter
Adjunct Professor Kjell Moljord

Laboratory personnel:
Engineer Karin Wiggen Dragsten
Part time in 2011: Inger Marie Bjørnevik, Erland Strendo, Stefan Kjærnli

Doctoral students 2011/2012:
Farbod Dadgar
Hassan Jamil Dar
Asmira Delic
Ilya Gorelkin
Daham Gunawardana
Fatemeh Hayer
Fan Huang
Saima Sultana Kazi
Andreas Helland Lillebø
Fengliu Lou
Oana Mihai
Navaneethan Muthuswamy
Tayyaba Noor
Eleni Patanou
Xuyen Kim Phan
Paul Radstake
Shreyas Pandurang Rane
Miroslav Surma
Ingvild Tronstad
Nikolaos Tsakoumis
Charita Udani
Nicla Vicinanza
Andrey S. Volynkin
Alexey Voronov
Georg Voß

Postdoctoral fellows 2011/2012:
Bjørn Christian Enger
Nina Hammer
Ingeborg-Helene Svenum
Estelle Vanhaecke
Espen Wangen
Dung Trung Tran
Fan Huang
Tiejun Zhao
Jun Zhu
Jia Yang
Sara Boullosa Eiras

Visitors:
Javier Fermoso Dominguez
Juan Du
Cristian Ledesma Rodrigues
Seyedali Hosseini
Peng Cui

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
Frode Sundset

SINTEF Materials and Chemistry
Kinetics and Catalysis Research Team

Administration:
Research Manager Torbjørn Gjervan
Senior-/Project Secretary Berit Broli

Research scientists:
Research Scientist Håkon Bergem
Research Scientist Svatopluk Chytil
Research Scientist Odd Asbjørn Lindvåg
Research Scientist Hilde Bjørgan
Research Scientist Rune Myrstad
Senior Scientist Rune Lødeng
Professor II Emeritus Odd A. Rokstad

Laboratory personnel
Engineer Camilla Otterlei
Engineer Marianne Aune

Third row: Fan Huang, Georg Voß, Alexey Voronov, Bjørn Christian Enger, Daham Sanjaya Gunawardana, Rune Myrstad, Edd A. Blekkan, Anders Holmen, Odd Asbjørn Lindvåg, Rune Lødeng, Håkon Bergem, Ilya Gorelkin, Paul Radstake.

Second row: Seyedali Hosseini, Camilla Otterlei, Karin Wiggen Dragsten, Marianne Aune, Javier Fermoso Dominguez, Gjervan, Torbjørn, Fengliu Lou, Eleni Patanou, Hilde Bjørkan, Andrey S. Volynkin, Hassan Jamil Dar, Ingeborg-Helene Svenum, Hilde Venvik.

First row: Ingvild Tronstad, Tayyaba Noor, Charitha Udani, Farbod Dadgar, Andreas H. Lillebø, De Chen, Jun Zhu, Jia Yang, Sara Boullosa Eiras, Juan Du, Nicla Vicinanza, Nikolaos Tsakoumis.

Not present: Magnus Rønning, Trung Dung Tran.

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

- **High Temperature Chemistry**
  - Free radical chain reactions
  - Partial oxidation of methane and NGL compounds

- **Environmental Catalysis**
  - Sulfur reduction by hydrotreating
  - 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) modeling

- **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
- CSTR reactors
- Transient kinetics (Steady-State Isotopic Transient Kinetic Analysis)
- Multireactor system for CNF synthesis

❖ Catalyst Preparation Laboratory

- Spray drier

❖ Catalyst Characterization

- Surface area (BET), porosity and pore size distributions
- Chemisorption
- Temperature programmed methods such as TPR, TPO and TPD
- TGA and DSC
- Raman and IR spectroscopy
- Acidity determination by TPD
- UV-VIS
- 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.

Highlights from the Activities in 2011

- Nine candidates completed their PhD degrees in 2011: Xuyen Kim Phan, Fatemeh Hayer, Shreyas Pandurang Rane, Fan Huang, Oana Mihai, Jia Yang, Nikolaos E. Tsakoumis, Kazi Saima Sultana and Navaneethan Muthuswany. The titles of the dissertations and pictures of the candidates/committes/supervisors are enclosed.
- The main research laboratories of the Catalysis Group have been completely renovated during the last two years (two flooors in Chemistry hall D). The completion of the work was celebrated with an official opening with representatives from NTNU and SINTEF and a seminar where a large fraction of past PhD-students in the group attended. The program is enclosed. The laboratories will be in full operation during Spring 2012.
- The occasion of the official retirement of professor Anders Holmen was marked in two ways: An international seminar in Trondheim with approx. 100 participants and invited lectures from a number of leading scientists. The program is enclosed. A special issue of Topics in Catalysis entitled Catalysis for Clean Energy (Guest editors: Blekkan, Chen, Rønning, Venvik) with 28 contributions by friends and colleagues of professor Holmem from all across the world.
- The Group participates in inGAP (Innovative Natural Gas Processes and Products) – a Centre for Research–based Innovation (SFI) with participation from the University of Oslo, SINTEF, NTNU, Statoil, Inéos, and Halldor Topsøe AS. The centre was evaluated with good results in 2011 and extended for 3 more years.
- The Group is established as a Gemini centre (twin research centre).
- 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 cleaning. The Group is also coordinating a EU-FP7 project on development of new metal-free catalysts to replace noble metal catalysts in strategic reactions.
- Members of the Group participate in EU networks like the Eurokin network and BRISK (Biofuels Research Infrastructure for Sharing Knowledge) and in large national research programs such as GASSMAKS, NANOMAT, PETROMAKS, RENERGI, KOSK

Ph. D Candidates and Postdoctoral Projects

Deactivation of Cobalt based Fischer – Tropsch synthesis catalysts

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

The Fischer-Tropsch synthesis (FTS) 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 FTS. 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 deactivation of FTS 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 into advanced *in-situ*/*operando* characterization studies. 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 monitoring of the active sites is very challenging. We have optimized a quartz capillary *in-situ* cell in order to combine photon based techniques at realistic FT conditions. The cell has been successfully tested at the Swiss-Norwegian beam lines (SNBL - ESRF, Grenoble). The XAS and XRPD techniques were combined for the *in situ* characterization of the catalyst with simultaneous product analysis. 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 2011:

N. E. Tsakoumis, A. Voronov, M. Rønning, Ø. Borg, E. Rytter, A. Holmen. *An operando study of Co-based Fischer-Tropsch synthesis catalysts*. Poster presentation, EuropaCatX: Catalysis – across the disciplines, Glasgow, Scotland, 28 August – 02 September 2011.

Financial support:

The Norwegian Research Council through *in*GAP project (Innovative Natural Gas Processes and Products) and the Dept. of Chemical Engineering, NTNU.

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 2011:

1. J. Yang, D. Chen, and A. Holmen. *Understanding the kinetics and Re promotion of carbon nanotube supported cobalt catalysts by SSITKA.* Catalysis Today: doi: http://dx.doi.org/10.1016/j.cattod.2011.10.026.

2. X. Phan, J. Yang, H. Bakhtiary-Davijnay, R. Myrstad, H. Venvik and A. Holmen. *Studies of macroporous structured alumina based cobalt catalysts for Fischer-Tropsch synthesis.* Catal. Lett., 141 (2011) 1739.
3. J.M.G. Carballo, J. Yang, A. Holmen, S. García-Rodríguez, S. Rojas, M. Ojeda and J.L.G. Fierro. *Catalytic effects of ruthenium particle size on the Fischer–Tropsch Synthesis*. J. Catal., 284 (2011) 102.
4. 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.* Topics in Catalysis, 54 (2011) 768.

Financial support:
The Norwegian Research Council through KOSK II and the Department of Chemical Engineering, NTNU.

New approach to metal dusting corrosion

Ph.D. candidate: Daham Sanjaya Gunawardana Panditha-Vidana
Supervisors: 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 materials into fine dust like particles. It constitutes a problem in the chemical and petrochemical industries, where metals and alloys extensively exposed to carbon-supersaturated gaseous environment (where carbon activity is very high; $a_C > 1$) with low partial pressures of oxygen or steam at elevated temperatures (300 ^{o}C and above). Metal dusting carries significant cost which is associated with application of certain precautionary measures and ultimate replacement of certain process unit and equipment.

The overall objective of this study is to obtain better understanding of the initial stages in metal dusting corrosion, *i.e.* the initiation of the carbon formation. This is done by preparing different surface oxides of a representative alloy, which is then exposed to high carbon activity (a_C>1) gas atmosphere at high temperature. This is combined with detailed characterization before and after the exposure in order to find a relationship between the structure and composition of the alloy surface and its propensity to form solid carbon. Since the initial carbon formation as well as the progress of the metal dusting is affected by numerous parameters, including even the flow pattern and material stress as well as the more obvious structure and composition of the exposed alloy surface, temperature, pressure, and composition of the gas stream, great

care has been taken to chose consistent experimental procedures that treat one parameter at the time.

Ni-based industrial alloy (Inconel 601) samples are prepared in a laboratory setup under controlled conditions. Each sample is subjected oxidation treatment before CO exposure. The surface and bulk morphology and composition of oxidized as well as CO exposed samples are investigated by optical microscopy, SEM and AES. The results show that both the structure and the composition of the oxide are important to its integrity when subjected to a carbon-supersaturated gas. A higher initial carbon formation appears to be associated with inclusion of Ni and/or Fe species in the surface oxide, which composition as well as structure is dependent on the oxidation conditions. Next, the assessment of mass change under relevant reaction conditions will be applied to obtain the rate of metal dusting, and techniques such as TEM and Raman spectroscopy techniques will be applied to further investigate carbon formation.

Presentations in 2011:

1. P.V.D.S. Gunawardana, Hilde Venvik: *Investigation of the initiation of metal dusting corrosion*, Oral presentation in InGAP seminar, 01st Dec., 2011, Trondheim, Norway.
2. P.V.D.S. Gunawardana, J.C. Walmsley, Hilde Venvik: *Investigation of the initiation of metal dusting corrosion*, Poster presentation in InGAP seminar, 01st Dec., 2011, Trondheim, Norway.
3. P.V.D.S. Gunawardana, J.C. Walmsley, Hilde Venvik: *Metal dusting corrosion initiation in conversion of natural gas to synthesis gas*, Oral presentation in 2nd Trondheim Gas Technology Conference 2011, 2–3rd November 2011, Trondheim, Norway.

Financial support:
The project is funded by the research council of Norway through Innovative Natural Gas Processes and Products (*in*GAP).

Catalyst formulations for use in microstructured reactors for conversion of synthesis gas to liquids

Ph.D-Candidate: Xuyen Kim Phan
Supervisors: Profs Anders Holmen and Hilde J. Venvik

Potential natural gas reserves in the world are more than 6000 trillion cubic feet. However, approximately 25% of these gas reserves are located offshore with no economic feasibility to be produced, transported and sold. This calls for finding

solution for utilization of the resources. Exploiting offshore natural gas presents challenges that possibly could be overcome by offshore conversion of gas to liquids (e.g. methanol, synthetic gasoline/diesel (Fischer-Tropsch technology) or dimethyl ether (DME)). For offshore gas-to-liquids (GTL), the production unit would require compact, efficient, robust, lightweight, reliable and safe technologies. Microstructured reactors may present an interesting potential for offshore GTL technology. Development of catalysts for use in microstructured reactors is an important part to get a more viable technology. The purpose of the present work is preparation, characterization and performance of different catalyst formulations for use in microstructured reactors for conversion of synthesis gas to liquids.

The Cu-based coatings were prepared using different techniques: slurry coating of $CuO/ZnO/Al_2O_3$ obtained via 2-stage co-precipitation, sol-gel coating of Al_2O_3 followed by Cu-Zn impregnation, colloid coating of Al_2O_3 followed by Cu-Zn impregnation, and colloid coating of Al_2O_3 followed by deposition-precipitation of Cu-Zn. The coated monoliths were characterized (XRD, BET, N2O titration) and studied in the methanol synthesis reaction at 80 bar.

The stacked foil microstructured reactor (SFMR) for producing methanol from synthesis gas could be demonstrated at high pressure, proved up to 80 bar. It is furthermore shown that two different active catalyst foil coatings could be prepared and tested, Pd/CeO_2 and $CuO/ZnO/Al_2O_3$. The performance of the catalyst-reactor systems could also be compared to that of a laboratory scale fixed-bed reactor (FBR) containing catalyst particles of similar composition.

MPS-Al_2O_3 support was successfully synthesized from Al_2O_3 nanoparticles and sacrificed PS beads. The structure obtained contained uniformly spherical pores which were interconnected throughout the whole sample. The support was confirmed having α-phase alumina, but had relatively higher water adsorption capacity than that of a conventional α-Al_2O_3, giving a higher Co dispersion of Co/MPS-Al_2O_3 than that of Co/α-Al_2O_3. The SSITKA studies showed that this higher dispersion helped improving rate of reaction, comparable with the Co/γ-Al_2O_3 catalyst, but without sacrificing the selectivity as compared with α-Al_2O_3. The MPS-Al_2O_3 supported cobalt catalyst hence seems to combine the advantages of both Co/α-Al_2O_3 and Co/γ-Al_2O_3 catalysts.

Publication and presentation in 2011

1. Xuyen K. Phan, Hamidreza Bakhtiary-Davijany, Rune Myrstad, Janina Thormann, Peter Pfeifer, Hilde J. Venvik, and Anders Holmen. *Preparation and performance of Cu-based monoliths for methanol synthesis*. Appl. Catal. A: Gerneral. 405 (2011) 1-7.

2. Xuyen K. Phan, Jia Yang, Hamidreza Bakhtiary-Davijany, Rune Myrstad, Hilde J. Venvik, Anders Holmen. *Studies of Macroporous structured Alumina based Cobalt Catalysts for Fischer-Tropsch Synthesis*. Catal. Lett. 141 (2011) 1739-1745.

3. H. Bakhtiary, F. Hayer, X.K. Phan, R. Myrstad, H.J. Venvik, P. Pfeifer, A. Holmen: Characteristics of an Integrated Micro Packed Bed Reactor-Heat Exchanger for Methanol Synthesis from Syngas. Chem. Eng. J. 167 (2011) 496-503.
4. Hamid Bakhtiary Davijany, Fatemeh Hayer, Xuyen Kim Phan, Rune Myrstad, Peter Pfeifer, Hilde J. Venvik, Anders Holmen: Performance of a multi-slit packed bed microstructured reactor in the synthesis ofr methanol: Comparison with a laboratory fixed-bed reactor. Chem. Eng. Sci. **66** (2011) 6350-6357.
5. Hamid Bakhtiary Davijany, Farbod Dadgar, Fatemeh Hayer, Xuyen Kim Phan, Rune Myrstad, Hilde J. Venvik, Peter Pfeifer, Anders Holmen: Analysis of external and internal mass transfer at low Reynolds numbers in a multi-slit packed bed microstructured reactor for synthesis of methanol from syngas. Submitted.
6. X.K. Phan, J. Walmsley, H. Bakhtiary-Davijany, R. Myrstad, P. Pfeifer, A. Holmen, H. Venvik: Characterization and Performance of Pd/CeO_2 Catalysts as a Powder in Fixed-bed Reactor and as a Coating in a Stacked Foil Microreactor for Methanol Synthesis. Poster. EuropaCat X. August 28 – September 2011, Glasgow, Scotland.

Financial support:
The partners of the Remote Gas project (Statoil ASA, UOP, Bayerngas Norge, Aker Solutions, DNV and the Research Council of Norway), performed under the strategic Norwegian Research program PETROMAKS and the Department of Chemical Engineering, NTNU.

Palladium based membranes in catalytic reactions

PhD candidate: Nicla Vicinanza
Supervisors: Professor Hilde Johnsen Venvik, Dr. Scient. Rune Bredesen and Dr. Thijs Peters, SINTEF

Palladium-based membranes have long been subject of many studies due to their high hydrogen permeability and selectivity, and because they are potential candidates for use in membrane reactors. The main disadvantage is that Pd is expensive, and the material costs are proportional to the thickness. SINTEF has developed a technology to produce Pd alloy membranes with thickness down to 1-2 μm that significantly improves flux and reduces material costs .

The main aim of this project is development of thin Pd-alloy membranes with improved thermal stability, sulphur resistance and resistance to flux inhibition by CO, and their integration in reactors under water-gas shift and steam reforming conditions. Attention is devoted to choose the best

composition, fabrication parameters and pretreatment procedure to improve hydrogen permeation. Following an extensive laboratory renovation, permeation measurements are being performed in a renewed and updated experimental setup. Changes in the topography and chemical composition of the membrane surface will be analyzed using AFM and XPS, as well as other suitable techniques. The oxidation of the Pd-alloy surface will be investigated using thermo-gravimetric analysis (TGA). SINTEF Materials and Chemistry is manager of the project, with the Colorado School of Mines as an international partner.

Publications:
Rune Bredesen, Thijs A. Peters, Marit Stange, Nicla Vicinanza and Hilde J. Venvik: *Palladium-based Membranes in Hydrogen Production*, in Membrane Engineering for the Treatment of Gases: Gas-separation Problems Combined with Membrane Reactors, Chapter 11 DOI:10.1039/9781849733489-00040

Financial support: Research Council of Norway (RENERGI programme, Contract No. 190779/S40) and Statoil ASA through the NTNU-SINTEF Gas Technology Centre.

Direct Synthesis of Dimethyl Ether in Microstructured Reactors

PhD candidate 2007-2011: Fatemeh Hayer
PhD candidate 2011- : Farbod Dadgar
Supervisors: Professor Hilde J. Venvik, Professor Anders Holmen

Dimethyl ether (DME) has promising potential as an alternative fuel and can be produced from wide range of feedstock such as natural gas, coal and biomass. The direct synthesis of DME from synthesis gas is highly exothermic and proper temperature control to avoid run-away is important. So-called microstructured reactors could provide the key to intensify compact production of DME, and the project focused on the performance assessment of integrated micro packed bed reactor-heat exchangers (IMPBRHE) for this purpose.

Three different IMPBRHEs for direct DME synthesis over physical mixtures of CuO-ZnO-Al2O3 and γ-Al2O3 catalysts were investigated experimentally as well as by mathematical modeling and simulation. The reactors had different number of reaction slits or different slit dimensions, and they either contained equally spaced pillars over the complete slit or at the inlet and outlet only.

The measured pressure drop (at 20 °C) was always small (<0.12 bar) relative to the total pressure (50 bar) and showed linear dependence with GHSV

in agreement with a predicted laminar flow regime for Re=0.1-2. A narrow residence time distribution (RTD) was estimated by dispersion analysis, i.e. investigations of the Peclet and Bodenstein numbers. Careful temperature measurements inside the slits, along the reactor housing and at oil inlet and outlet, confirmed that the reaction slit temperature is mainly controlled by the oil heat exchange to give a practically uniform temperature profile over reactors for set inlet oil temperatures of 220-320 °C. The micro packed beds were found to be free from internal as well as external mass transfer limitations, as confirmed by no significant change in the CO conversion and DME yield for different catalyst particle sizes, no effect of varying the linear gas velocity, and no effect of manipulating reactant diffusion coefficient.

The performance of a single slit micropacked bed reactor in direct DME synthesis was represented by a 3D pseudo homogeneous reactor model, incorporating kinetic expressions for the methanol synthesis and methanol dehydration reaction from literature. The concentration and temperature distribution in the reaction slit was estimated by assuming a uniform wall temperature. The model was adopted at low Reynolds numbers, i.e. small catalyst particles and long residence times. The reactor simulation showed good agreement with experimental results and could be further developed to assess the potential of microstructured packed bed reactors for intensification of conventional large-scale processes.

Publications and presentations

1. F. Hayer, H. Bakhtiary-Davijany, R. Myrstad, H.J. Venvik, P. Pfeifer, A. Holmen, *Synthesis of Dimethyl Ether from Syngas in a microchannel reactor - simulation and experimental study.* Chem. Eng. Journal 167 (2011) 610–615
2. F. Hayer, H. Bakhtiary-Davijany, R. Myrstad, A. Holmen, P. Pfeifer, H. J. Venvik. *Modeling and Simulation of an Integrated Micro Packed Bed Reactor-Heat Exchanger Configuration for Direct Dimethyl Ether Synthesis*. Topics in Catalysis 54 (2011) 817-827. Special issue honoring Prof. Anders Holmen's 70th birthday.
3. H. Bakhtiary-Davijany, F. Hayer, X. K. Phan, R. Myrstad, P. Pfeifer, H. J. Venvik, A. Holmen. *Performance of a multi-slit packed bed microstructured reactor in the synthesis of methanol: Comparison with a laboratory fixed-bed reactor*. Chem. Eng. Sci. 66 (2011) 6350–6357.
4. H. Bakhtiary-Davijany, F. Hayer, X. K. Phan, R. Myrstad, H. J. Venvik, P. Pfeifer, A. Holmen: *Characteristics of an Integrated Micro Packed Bed Reactor-Heat Exchanger for methanol synthesis from syngas.* Chem. Eng. Journal 167 (2011) 496-503.
5. F. Hayer, H. Bakhtiary-Davijany, R. Myrstad, H.J. Venvik, P. Pfeifer, A. Holmen, *Characteristics of integrated micro packed bed reactor-heat*

exchanger configurations in the direct synthesis of dimethyl ether, Submitted to Chemical Engineering and Processing: Process Intensification Journal
6. H. Bakhtiary-Davijany, F. Dagagar, F. Hayer, X. Kim Phan, R. Myrstad, H. J. Venvik, P. Pfeifer, A. Holmen. *Analysis of external and internal mass transfer limitations at low Reynolds numbers in a multi-slit packed bed microstructured reactor under real methanol synthesis operating conditions.* Submitted to Industrial and Engineering Chemistry Research (2011)
7. H. J. Venvik, F. Hayer, H. Bakhtiary Davijany, A. Holmen, P. Pfeifer, R. Dittmeyer, R. Myrstad. *Direct synthesis of dimethyl ether in microstructured reactors*. Oral presentation, EuropaCat X; 2011-08-28 - 2011-09-02
8. F. Dadgar, H. Bakhtiary Davijany, P. Pfeifer, R. Myrstad, A. Holmen, H. J. Venvik,. *Assessment of mass transfer limitations and catalysts deactivation for methanol synthesis in a microstructured reactor.* Poster, OCMOL Colloquium on Chemical Reactor Engineering; 10-11 October 2011. Technical University Munich, Germany.

Financial support
The projects are funded by the Research Council of Norway under the GASSMAKS research program and Statoil ASA through the Gas Technology Centre (NTNUSINTEF).

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

PhD Candidate: Shreyas Rane
Supervisors: Prof. Anders Holmen, Prof Erling Rytter, Statoil 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 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.

Publication and presentations:

1. Shreyas Rane, Øyvind Borg, Erling Rytter, Anders Holmen. *Relation between hydrocarbon selectivities, activity and particle size for alumina supported cobalt based catalysts in Fischer-Tropsch synthesis*. Submitted.
2. Saka Zarubova, Shreyas Rane, Jia Yang, Yingda Yu, Ye Zhu, De Chen, Anders Holmen *Fischer-Tropsch synthesis on Hierarchically Structured Co-Nanoparticles/Carbon Nanofibers/Carbon-felt Composites*. ChemSusChem 4 (2011) 935-942
3. A. Lillebø, C. Balonek, S. Rane, E. Rytter, E.A. Blekkan, A.. Holmen: *Fischer-Tropsch biomass to liquids, effect of LI, Na, K, and Ca on Cobalt catalysts.* 1st International Congress on Catalysis for Biorefineries (CatBior 2011). October 2-5 2011. Malaga, Spain.

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

New concepts in the catalytic dehydrogenation of propane

PhD student: Ilya V. Gorelkin
Project leader: Professor Edd A. Blekkan

The production of light alkenes (C2-C4) 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. In this project we study fundamental and applied issues in propane dehydrogenation, mainly the development of a new concept in process heating. The concept is 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.

Presentations 2011:

1. I. V. Gorelkin, E.A. Blekkan. Concepts and models of the catalytic dehydrogenation of propane. 22nd North American Catalysis Society Meeting, Detroit, USA, June 5-10, 2011.
2. I. V. Gorelkin, E.A. Blekkan. Concepts and models of the catalytic dehydrogenation of propane. EuropaCat X, Glasgow, Scotland, Aug 28 – Sept 2, 2011.

Financial support:
The Gassmaks program from The Research Council of Norway.

Microcalorimetry and microkinetics of heterogeneous catalysts.

PhD 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 modeling 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 heat transferred per unit time is 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 directly from the reduction into the calorimeter in order to start the adsorption process with the chosen probe gas. In the present work microcalorimetric results are used to eliminate errors and to assure better fitting of the computational techniques with the Fischer-Tropsch catalysts.

Presentations and publications

1. E. Patanou, De Chen, E.A. Blekkan. Microcalorimetric studies on cobalt supported catalysts for Fischer – Tropsch synthesis. EuropaCat X, Glasgow, Scotland, Aug 28 – Sept 2, 2011.
2. E. Patanou, E.A. Blekkan. Hydrogen adsorption on supported cobalt catalysts for the Fischer-Tropsch synthesis studied by microcalorimetry. Norwegian Chemical Society Annual Meeting, Lillestrøm , Norway 2011.

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

3D Carbon/polyaniline Nanostructures for Energy Storage

PhD candidate: Fan Huang
Supervisor: Prof. De Chen

The project in the period of 2011 has moved from the examination of the *in-situ* polymerization of different conducting polymers on carbon nanostructures in year 2009 to systematically investigating the electrochemical performance of PANI/CNT as electrode material in supercapacitors and cathode material in Li-batteries.

A systematic study on the composite materials containing various loadings of PANI has shown: The specific capacitance based on PANI phase reached 1100 F/g when the PANI film is thinner than 11 nm, which was approaching the limited value that PANI could provide. The rate capability and cycling stability were also influenced by the coating thickness of PANI. A principle of designing the optimal microstructure of the composite materials towards high specific power and specific energy and good cycling stability was developed: high loading and thin layer of PANI should be obtained at the same time.

This principle was realized by depositing a 9 nm of PANI on much smaller ACNTs (9 nm in diameter) which were facilely synthesized on household aluminum foil. A highly flexible symmetric supercapacitor was built and demonstrated, simulating the harsh working conditions such as bending and twisting. Such cost-effective and highly flexible supercapacitors provide a promising future in the industrial manufacturing and applications.

Publications in 2011

Fan Huang, Fengliu Lou and De Chen: *Exploring Full Potential of ACNT@polyaniline Arrays on Household Al as Highly Flexible and Cost-Effective Supercapacitors*. ChemSusChem, 2012. On line.

Estelle Vanhaecke, Fan Huang, YingdaYu, Magnus Rønning, Anders Holmen, De Chen: *Catalytic consequence of the interface between iron catalysts and foils in synthesis of aligned nanocarbons on foils.* Topics in Catalysis 54, 986-997, 2011.

Financial support:
The Norwegian Research Council (NFR)

Insulating liquids

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

High voltage transformers are insulated with mineral oil and solid cellulose (paper wrapped around the copper windings). Failures (short-circuits), caused by deposits on the windings in these transformers have dramatic consequences for everyday life and industry. To prevent failures it is important to understand how the insulating materials work in the transformer. By the use of traditional analytical methods such as titration, as well as introducing new techniques such as QCM (Quartz Crystal Microbalance) and microcalorimetry, we try to understand the reactions and effects of the chemicals in the insulating materials. Corrosion and formation of copper sulphide in transformer insulations and oxidation of insulating liquids (including alternative, environmentally friendly liquids), are the main areas of study. The project is a part of the KMB project Thermal and electromagnetic performance of transformers, which is a joint effort between NTNU, SINTEF Energiforskning AS, Statnett, Hafslund, Statkraft, EDF, ABB, Nynäs, Siemens, NVE and The Research Council of Norway.

Publications and presentations

1. I. Tronstad, M.-H. Ese, E.A. Blekkan. Isothermal microcalorimeter as a tool for studying oxidation stability of insulating liquids. Submitted, IEEE Transcations.

Financial support:
Statnett, Hafslund, Statkraft, EDF, ABB, Nynäs, Siemens, NVE and 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, H2S), 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 2011:

1. Espen Standal Wangen, Edd A. Blekkan. *Catalytic conditioning of bio-syngas*. GreenSyngas workshop, Güssing, Austria 23. February 2011.
2. Espen Standal Wangen, Amin Osatiashtiani, Edd A. Blekkan, *Reforming of syngas from biomass gasification: Deactivation by tar and potassium species*. Topics in Catalysis 54 (2011) 960-966.

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

Conversion of synthesis gas from biomass to liquid fuels by the Fischer-Tropsch synthesis

PhD candidate: Andreas Helland Lillebø
Post. doc: Bjørn Christian Enger
Supervisor/Project director: Profs. Anders Holmen & Edd A. Blekkan

The main objective is to study CO hydrogenation (Fischer-Tropsch synthesis) on modified Fischer-Tropsch catalysts using synthesis gas (CO + H_2) derived from biomass. The technology for conversion of biomass to liquid fuels (BTL) is similar to the technology for gas to liquids (GTL) and the objective is to focus on the differences and challenges specific to biomass derived synthesis gas. In particular, biomass derived synthesis gas contains large amounts of contaminants like alkali, H_2S, COS, NH_3, HCN, dust and tars. Cobalt based Fischer-Tropsch catalysts are very sensitive to contaminants and ppm levels of contamination is known to modify the hydrocarbon selectivity and cause catalyst deactivation. It is possible with state-of-art technology to remove the contaminants down to acceptable levels. However, the economic risk related to a trip or failure, where a breakthrough of contaminants reaches the catalyst, is very high because of the high replacement cost for the catalyst. Thus, knowing the severity of and managing this risk as well as designing catalysts which are more tolerant to contaminants will help to reduce the commercial risk for BTL.

Publications and presentations in 2011:

1. Bjørn Christian Enger, Åse-Lill Fossan, Øyvind Borg, Erling Rytter, Anders Holmen, *Modified alumina as catalyst support for cobalt in the Fischer Tropsch synthesis*, J. Catal. 284 (2011) 9-22.
2. Bjørn Christian Enger, Vidar Frøseth, Erling Rytter, Anders Holmen, *SSITKA studies of cobalt catalysts on modified aluminas in the Fischer Tropsch synthesis*, submitted.
3. Bjørn Christian Enger, Rune Lødeng, Anders Holmen, *On the nature of elementary reactions from methane to hydrogen over transition metals.* Int. J. Hyd. Energy (2012) In press.
4. Bjørn Christian Enger, Anders Holmen, *Review: Nickel and Fischer Tropsch synthesis.* Catalysis Reviews Science & Engineering (2012) Accepted.
5. Bjørn Christian Enger: *Biomass to liquids (BTL).* Oral presentation. VISTA-dagen at Rotvoll, 13 September 2011.

6. Bjørn Christian Enger, Vidar Frøseth, Erling Rytter, Anders Holmen: *Effects of Zn during SSITKA studies of Co-Re/γ-Al_2O_3 catalysts in the Fischer-Tropsch synthesis:*Poster. Europacat X, 27 August – 3 September 2011, Glasgow, Scotland.

Financial support:
The Norwegian Academy of Science and Letters (VISTA), Statoil, SINTEF, NTNU (Gas Technology Center) and the Norwegian Research Council through NRC project 19073- Biomass to liquid fuels.

Study of the deactivation mechanisms on Co-based Fischer-Tropsch catalysts under 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.

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. Many parameters have a serious influence to the FT catalyst deactivation, so it is essential to involve several characterization techniques in order to distinguish influence of the various external conditions and define the separate deactivation routes.

Modulation excitation spectroscopy (MES) is a group of techniques which allow to detect and monitor the dynamic behavior of species involved in a chemical reaction. In combination with suitable in situ spectroscopic techniques it becomes a powerful tool for studying catalytic reactions and investigating catalysts under realistic working conditions.

The MES technique was coupled with X-ray absorption spectroscopy (XAS) in order to investigate catalyst behavior in the FT reaction. A quartz capillary microreactor was used as a micro catalytic fix-bed reactor. Several gases and gas mixtures were exposed to the sample. We have obtained detailed

information about surface behavior on a cobalt FT catalyst during red-ox treatment, CO exposure, and also FT synthesis.

The purpose of the project is to obtain 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.

Financial support:
The project is funded by NTNU and the Norwegian Research Council (NFR) through the InGAP centre.

Photocatalytic fuel production by reforming of hydrocarbons and CO_2

Ph.D. candidate: Punchi Patabandige Charitha Udani
Supervisor: Professor Magnus Rønning

The photocatalytic fuel production using solar energy is a challenging research topic which has received much attention in recent years for its potential to provide H_2 as a clean and renewable energy carrier even on a large scale. This can be done with the use of several methods including water photosplitting and even more efficiently, by photoreforming of organic compounds, including methane, alcohols, aldehydes and organic acids to yield H_2 and CO_2 mixtures.

The increasing levels of CO_2 in the atmosphere have now become a global environmental issue because of the green house effect. There have been various approaches not only for recycling of this green house gas but also for an efficient production of fuel alternatives. It is reported that CO_2 can be re-introduced in the energy cycle by photoreforming into fuels such as CO, CH_4, CH_3OH, and H_2 .

The project is mainly focused on producing fuel alternatives with the use of an artificial solar light source and various photocatalysts. Various hydrocarbons, catalyst synthesis methods and catalysts formulation will be used, comparing noble metals with transition metals and combinations of these with the aim to prepare cost-effective catalyst systems. To investigate the crystal phase changes and morphology changes, the photocatalysts will be subjected to characterization also after exposure to the reaction conditions and as far as possible, *in situ* characterization when the catalysts are working.

Financial support:
The project is funded by strategic funding, NTNU.

The role of carbon in catalytic dehydrogenation of hydrocarbons

PhDcandidate: Andrey S. Volynkin
Supervisors: Prof. Edd A. Blekkan, Prof. Magnus Rønning

Carbon can play different roles in catalytic dehydrogenation (DH) of light hydrocarbons. While coke deposition deactivates dehydrogenation catalysts, carbon (with oxygen containing functional groups) can also be catalyst on its own for other dehydrogenation reactions. Another aspect of carbon in dehydrogenation is studies of carbon as support for the active metal. Oxygen containing sites can anchor metal nanoparticles and therefore assist the deposition of metal on carbon. Subsequent reduction in H_2 atmosphere removes the oxygen containing sites and reduces the active metal, making the catalyst able to dehydrogenate hydrocarbons. Metal-support interaction is an important parameter in catalysis and the way Pt and Pt-Sn will interact with carbon support (graphite, active carbon, carbon nanofibres and carbon nanotubes) and the implication of this interaction on the selectivity for DH can be difficult to predict. Carbon nanofibres and carbon nanotubes are not practical catalysts for dehydrogenation-reactions, but provide interesting properties as model systems.
The aim of this project is to improve understanding of effects of carbon on catalytic dehydrogenation of light alkanes, especially:

- Synthesis of carbon materials and study of their catalytic properties.
- Study of dehydrogenation properties of Pt and Pt-Sn metal catalysts deposited on synthesized carbon materials (graphite, carbon nanofibres and carbon nanotubes). Investigation of metal-support interaction.
- Study of coke formation on Pt and Pt-Sn supported on carbon. Use of different spectroscopic techniques to discriminate carbon from support and carbon from coke formed during catalytic tests. Those techniques include Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy and Terahertz time-domain spectroscopy (THz-TDS).

Financial support:
Strategic funding, NTNU. Phd-pool , The Research Council of Norway

Reactor design and simulation for oxidative dehydrogenation of ethane to ethylene at atmospheric pressure.

PhD Student: Hassan Jamil Dar
Supervisor: Professor De Chen
Co-Supervisor: Professor 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, inducing numerous free radical reactions followed by immediate quench to freeze the reactions. By introducing oxygen to an ethane feed, ethylene can be produced via oxidative dehydrogenation of ethane (ODHE). 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 also reduces the reactor volume.
The goal of the project was to optimize the reactor design for the maximum yield of ethylene. The following objectives are achieved.

- A reliable kinetic model to describe the chemistry of oxidative dehydrogenation of ethane in the gas phase
- Analysis of different parameters (like temperature, C_2H_6/O_2 ratio) to get better yield is performed.
- The gas phase ODHE reaction is analyzed by means of the established kinetic model for ODHE, by using 1-D plug flow reactor model at isothermal condition, the path way analysis of the gas phase ODHE is performed, which describes the process limitation (low ethylene selectivity).
- Upper bound of the ethylene yield for the gas phase ODHE has been investigated

Presentation in 2011:
Hassan J. Dar, Sandro U. Nanot, Klaus J. Jens, Hugo A. Jakobsen, Elisabeth Tangstad, De Chen: Kinetic analysis of gas phase oxidative dehydrogenation for ethane to ethylene at atmospheric pressure. Poster. InGap- seminar: Trondheim, 01.12.2011.

Financial support:
The project is funded by NTNU and the Research Council of Norway (NFR) through the inGAP program.

Partial oxidation of methane.
Studies on mechanism and kinetics

PhD candidate: Oana Mihai
Supervisors: Profs Anders Holmen and De Chen

The mechanism and kinetics understanding of methane partial oxidation by chemical looping pathway is the purpose of this research project. The reaction is based on methane feeding by using lattice oxygen of perovskites oxides type LaFeO3 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. The iron-based 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. Different preparation methods of catalyst were used in order to get various averages of crystal sizes of $LaFeO_3$ perovskites.

The properties of surface and bulk oxygen are 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 has been to determine the surface reaction mechanisms.

Publications and presentations in 2011:

1. O. Mihai, D. Chen, A. Holmen, "*Catalytic consequence of oxygen of lanthanum ferrite perovskite in chemical looping reforming of methane*", Ind. Eng. Chem. Res. 50 (2011) 2613-2621
2. Oana Mihai, Miroslav Surma, De Chen, Anders Holmen: *Insight on the reaction mechanism understanding of methane partial oxidation: the effect of $LaFeO_3$ crystal size*. Submitted.

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

Microkinetic modeling of ethylene oxychlorination

Ph.D. candidate: Miroslav Surma
Postdoctoral Fellow: Dr. Jun Zhu
Supervisor: Prof. De Chen

Ethylene oxychlorination is an industrial process of great importance. Traditionally, $CuCl_2/Al_2O_3$ with different dopants (KCl, LaCl) is used as a catalyst for the reaction. Although many kinetic models have been proposed, none of them is able to describe the reaction over a wide temperature interval. The goal of this study was to carry out the series of transient catalytic experiments of particular reactions of the catalytic cycle with using the catalyst without any dopants.

First of all, $CuCl_2$ was reduced by ethylene to CuCl, then the Cu(I) was reoxidized by O_2 and finally, the HCl was used to regenerate the Cl content. Different reaction conditions (close to the industrial ones) were used and both the gas phase composition (by the means of MS) and the structure of the catalyst by *in situ* UV-vis spectroscopy were followed.

Langmuir-Hinshelwood kinetic models were delivered and it was found that the first reaction is the first order with respect to the available Cl concentration and the second reaction of the first order with respect to Cu(I) concentration. Absorption energy edge was calculated from fast scanning UV-vis reflectance measurements and the results were compared with MS data taken at the same time and the strong correlation of these results has been found. Furthermore, the importance of product desorption is proved by both techniques.

Publications and presentations in 2011:

1. Surma M., Fuglerud T., Lamberti C. and De Chen. *Transient kinetic investigation of Ethylene Oxychlorination*. Poster presentation in EUROPACAT X, August 28th to September 2nd, 2011,Glasgow. Scotland

2. Jun Zhu, De Chen. *Transient Kinetic Investigation of Ethylene Oxychlorination.* Oral presentation, inGAP Seminar, Trondheim, December 1st to 2nd, 2011

Financial support:

The project is funded by NTNU and the Norwegian research council through the InGAP center.

Dehydrogenation of NGL components at very short contact times

Ph.D. candidate: Paul B. Radstake
Supervisors: Profs. Anders Holmen and 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 is 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 is based on powdered Pt-Sn catalysts. Parameters to be investigated are mainly catalyst loading, atomic ratios of the different elements, type of support, synthesis procedures and catalyst precursors. The characterization is based on both physicochemical and spectroscopic techniques as well as the catalytic performance. Parameters within the catalytic testing experiments are investigated as well. These parameters include reaction temperature, gas flow rates and gas ratios.

Financial support:
The project is funded by the Norwegian research council (NFR), through the GASSMAKS program.

The State of Promotors in Fischer-Tropsch Catalysts

PhD candidate: Georg Voss
Supervisor: Prof. Magnus Rønning

Supported cobalt catalysts are widely studied because of their ability to convert synthesis gas in low temperature Fischer-Tropsch synthesis. These catalysts provide high activity, high selectivity to long chain paraffins and low water-gas shift activity. It is common practice to add a noble metal promoter to optimize the performance of the catalysts. Recently, more attention has been directed towards an understanding of the promotion to replace the noble metal promotors with less expensive alternatives. Promotion of the FT catalysts produces a variety of effects on the structure and catalytic performance. If this is due to the formation of bimetallic particles is a question which can only be answered by collecting more information about the state of the promoter metal under reaction conditions. Additionally, it has been found that alloy formation between catalyst-metal and promoter-metal changes the adsorption properties due to interactions in the outer shell orbitals. The detailed nanostructure, however, is unknown and further investigations are necessary.

This study focuses on the state of promotors in Fischer-Tropsch catalysts, especially at reaction conditions. The nature and location of the promoter itself is unclear which leads to the utilization of *in situ* techniques. The catalytic behaviour of Re and Ni promoted Co-FT catalysts is investigated using modulation excitation spectroscopy (MES) combined with X-ray absorption spectroscopy (XAS). MES allows for sensitive and selective detection and monitoring of the dynamic behaviour of species directly involved in the reaction. The set-up is capable of performing the experiments at industrially relevant FT conditions (20 bar, 210°C, H_2/CO atmosphere). Additionally, with resonant inelastic X-ray scattering (RIXS) element-selective studies of the electronic structure in the activated state are possible. Further studies will help identifying the electronic state of the promoter metal and its interaction with surrounding atoms.

Publications and presentations in 2011:

1. Georg Voss, M. Rønning. *The State of Promotors in Fischer-Tropsch Catalysts*. Poster. European Summer School "Energy and Materials of the Sun" 2011, Kerkrade, Netherland.
2. Georg Voss, M. Rønning: *The State of Promotors in Fischer-Tropsch Catalysts*. Poster. EuropaCat X**,** Catalysis – across the diciplines, Glasgow, Scotland, 28 August – 02 September 2011

Financial support:
The Research Council of Norway is acknowledged for financial support through the KOSK-II program. In addition, Statoil is kindly acknowledged for the support and co-operation in this project.

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

Postdoctoral Fellow: Ingeborg-Helene Svenum
Supervisors: Professor Hilde J. Venvik, Professor Manos Mavrikakis, Univ. of Wisconsin-Madison, USA, Professor Anne Borg, Dept. of Physics, NTNU

The manipulation of adsorption properties of catalysts and membranes in H_2/CO mixtures has been targeted by many researchers, and has relevance to natural gas conversion in general and hydrogen technology in particular. We discovered that CO inhibition of hydrogen transport through PdAg membranes was significantly reduced by membrane heat treatment in air. Analysis indicated changes in CO an H_2 heats of adsorption to play a role and surface spectroscopy

indicated segregation phenomena to be involved. The overall objective of the project is therefore to understand the response of Pd alloy surfaces to carbon monoxide and carbon dioxide the in presence of hydrogen by advanced characterization techniques in conjunction with detailed calculations, and to apply this knowledge to improved membranes, membrane reactors and catalysts. Our density functional theory (DFT) calculations showed that a $Pd_3Ag(111)$ membrane model surface is Ag rich in absence of adsorbates. If allowed to equilibrate, Pd atoms are pulled to the topmost surface layer upon adsorption of O, H or CO, making the $Pd_3Ag(111)$ surface Pd-dominated at the corresponding saturation coverages. The DFT studies further indicate that segregation within the uppermost layers of a $Pd_3Ag(111)$ surface may affect hydrogen adsorption, and hence transport.

The project partners are the NTNU Departments of Chemical Engineering and Physics and SINTEF Materials and Chemistry, with the University of Wisconsin-Madison as an international partner. The research is conducted through the postdoctoral fellowship and one PhD project at Dept. of Physics. Experimental investigations of binding energies, adsorption sites and surface species are targeted through modelling and experiments. The density functional theory calculations are performed using the DACAPO code, which is a state-of-the-art plane wave-pseudopotential implementation of DFT. Characterization is performed through high resolution, surface sensitive photoelectron spectroscopy and diffraction using high intensity, X-ray range, tuneable synchrotron radiation. Both model systems (single crystals) and membrane samples surfaces (sputtered Pd alloy thin films) are being studied.

Publications and presentations:

1. I.-H. Svenum, J.A. Herron, M. Mavrikakis, H.J. Venvik, Adsorbate-induced segregation in a PdAg membrane model system: $Pd_3Ag(111)$, Catalysis Today, In Press, doi: 10.1016/j.cattod.2012.01.007,
2. I.-H. Svenum, J.A. Herron, M. Mavrikakis, H.J. Venvik, Adsorbate induced segregation in Pd3Ag(111). Oral presentation. 10th International Conference on Catalysis in Membrane Reactors (ICCMR); 2011-06-20 - 2011-06-24.

Financial support:

The project is funded by the Research Council of Norway (KOSK II programme, Contract No. 197709/V30) and Statoil ASA through the NTNU-SINTEF Gas Technology Centre.

Nanostructured carbon-based reactors for catalytic water purification: Catalytic ozonation and nitrates reduction

Postdoctoral Fellowship: Dr. Estelle Vanhaecke, Dr. Fan Huang
Supervisor: Prof. Magnus Rønning

Catalytic ozonation is an innovative technology for the elimination of organic pollutants in water and wastewater. Carbon nanofibers are potential catalysts for ozonation due to the extended mesoporosity, which may have a very positive impact by decreasing the mass transfer resistance usually present in the microporous activated carbon. A continuous flow reactor for the structured catalysed consists of two columns connected to allow the water solution to circulate between the two. The first column is used to transfer the ozone from the gas phase into the liquid phase. The second column holds the structured catalyst and is used to contact the ozonated solution with the solid phase. Thus, there are two biphasic contact columns instead of a triphasic system.

The results show that the adsorption and the ozonation by itself are not effective to remove the oxalic acid. The best performance was observed for the untreated sample. The presence of oxygen-containing surface groups (present in high amount on the sample oxidized ACF/CF) has a detrimental effect. Therefore, the basic surface groups (mainly the electron-rich oxygen-free Lewis basic sites on the carbon basal planes) are the active sites for this reaction. The catalytic reduction of nitrates from ground water is becoming an environmental problem, especially for the drinking water. A promising catalyst system is the bemetallic Pd-Cu catalysts. A continuous flow reactor for the structured catalysts has been set up. In this experiment bimetallic catalysts supported on carbon nanofibers/graphite felt (CNFs/GF) are tested with continuous flow of H_2 and CO_2 within 3 hours of reaction and the reactant/product concentrations are measured by a UV/Vis spectrophotometer. Different parameters are studied: the nanostructure of the CNFs such as platelet CNFs/GF or fishbone CNFs/GF; the deposition technique for the catalysts; the reduction treatments of the bimetallic catalysts. We have also assembled a large-scale reactor capable of producing approximately 1 kg CNF per batch.

Presentations in 2011:

1. Estelle Vanhaecke, Kimete Osmani, Nina Hammer, De Chen, Magnus Rønning, *Towards optimized bi-metallic deposition on nanocarbon material supported for the reduction of nitrates in water,* Poster. EuropaCat X**,** Catalysis – across the diciplines, Glasgow, Scotland, 28 August – 02 September 2011
2. M.F.R. Pereira, J. Restivo, J.J.M. Órfão, E. Vanhaecke, M. Rønning, L. Kiwi-Minsker, S. Armenise and E. Garcia-Bordejé, *Catalytic ozonation of oxalic acid*

using carbon nanofibers on macrostructured supports, Water Sci. Tech. 10 (2011), in press

Financial support:
Monacat project, EU-FP7 Grant Agreement no 226347 (www,monacat.eu)

Multi-technique probing of catalytic reactions at real working conditions

Postdoctoral Fellow: Dr. Nina Hammer
Supervisor: Prof. Magnus Rønning

Heterogeneous catalysts are typically multiphase systems and the structure of the catalyst, i.e. their surface properties, defects, particle shapes and other structural properties, are most decisive for their performance. The structural and chemical state of the active species in the catalysts will depend on the process conditions. To understand how these properties can affect the catalytic performance is a major goal in catalysis research and hence the importance of in situ investigations of catalysts under real working conditions.

Synchrotron radiation techniques offer many of the necessary capabilities for probing the composition and structure of catalyst materials on the nanometer scale of the active particles. The techniques also allow for a study of the influence of the reaction conditions. These studies are essential in order to establish a basic understanding of catalytic reactions, the mechanisms of selectivity, activity and stability. A number of spectroscopic characterisation techniques have been adapted in recent years to study catalysts under working conditions. It is clear that, depending on its detection principle, each of these methods has its strength and limitations and will only give specific information. However, combining techniques such as XAS, XRD and Raman in situ provides a tool for studying a wide range of scientific problems which is much more powerful than the separate techniques.

The aim of this project is to use various in situ characterisation techniques to study the structure of catalytic systems under working conditions. The main focus will be on the XAS, XRD and Raman techniques and the experiments will be performed at the Swiss-Norwegian beamline. The experimental work is carried out in collaboration with other projects in our group.

Publications and presentations in 2011:
1. Nina Hammer, Karina Mathisen, Tina Zscherpe, De Chen, Magnus Rønning. *Effect of Pretreatment on Carbon-Supported Au/TiO2 Catalysts for Preferential Oxidation of CO*. Topics in Catalysis 54 (2011) 922-930
2. Estelle Vanhaecke, Kimete Osmani, Nina Hammer, De Chen Magnus Rønning, *Towards optimized bi-metallic deposition on nanocarbon material*

supported for the reduction of nitrates in water, EuropaCat X**,** Catalysis – across the diciplines, Glasgow, Scotland, 28 August – 02 September 2011

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

Fundamental understanding of catalyst nanoparticles by atomic scale chemical imaging

Postdoctoral Fellow: Dr. Dung Trung Tran
Supervisors: Prof. Magnus Rønning, Prof. De Chen, Dr. John Walmsley (SINTEF)

Fundamental study down to the atomic level is crucial for improving our understanding of catalysts and enhancing our ability for their rational design. The present project deals with exploring advanced TEM techniques such as aberration corrected microscopy and environmental TEM for imaging of composition and bonding. Elemental and valence sensitive imaging of Co nanoparticles and Pt based core-shell structured nanoparticles will be obtained by STEM combined electron diffraction and electron energy loss spectroscopy. The strain of the nanoparticles will be studied as a function of particle size and different supports in terms of catalytic performance in different reactions. The thickness and uniformity of the shell of core-shell structured nanoparticles are being studied by atomic imaging.

Recent work has demonstrated the value of detailed TEM analysis combined electron diffraction and EELS in nano oxide particles. The TEM at Trondheim is a Field Emission Gun (FEG) instrument equipped with STEM, X-ray composition analysis and EELS. This instrument can be used for detailed analysis of catalysts synthesized within the projects. The selected samples based on the results obtained in Trondheim TEM laboratory will be further investigated at DTU and Lehigh University. Lehigh is equipped with state-of-the art aberration corrected instruments. The ETEM at DTU has image aberration correction and a monochromator combined with EELS. The latter will be used to study the composition, bulk and surface atomic structure and chemistry and bonding down to the atomic scale. ETEM will be used to observe the samples under reducing conditions and in the presence of relevant gas atmospheres. This will allow atomic scale analysis under chemically active conditions without modification of the sample.

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

Calcium based CO2 acceptors for sorption enhanced steam reforming

Candidate: Kazi Saima Sultana
Supervisor: Prof. De Chen

Sorption-enhanced steam reforming (SESR) is a novel technology for reforming and in situ CO_2 removal using metal oxide acceptors such as Ca-based oxides. CO_2 capture capacity of natural Ca-based acceptors (e.g. dolomite, limestone) decline rapidly in multi-cycle carbonation/decarbonation processes. This project aims to develop Ca-based nano-acceptors with enhanced multi-cycle durability and CO_2 capture capacity. A comprehensive experimental study on synthesis and characterization of the nano-acceptors and their stability, reaction kinetics and performance in SESR has been conducted.

Spray drying and soft chemistry route are applied to develop high temperature Ca-based CO_2 acceptors. Spray drying technique is employed for the synthesis of Ca-based mixed oxides. Multi-cycle sorption stability of nano-CaO acceptors is enhanced by sol-gel and incipient wet impregnated coating. Ca-based acceptors are characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Brunauer-Emmett-Teller (BET) and Raman spectroscopy. The structural properties of the acceptors affect the CO_2 capture capacity, carbonation/decarbonation kinetics and stability. Acceptor performance is tested using a thermogravimetric (TG) analyzer and fixed bed reactor.

In multi-cycle carbonation/decarbonation, the nano-acceptors demonstrate relatively stable, reversible and high CO_2 uptake capacity compared to naturally occurring dolomite and $CaCO_3$ nano-particles. The synthetic nano-aceeptors have larger surface area and pore volume than the natural dolomite and $CaCO_3$. Thermogravimetric analyses (TGA) revealed that the mixed oxide nano-acceptors (40-100nm), CaCeZr, CaCe and CaZr show high-performance and stable CO_2 capture capacity up to 20 carbonation/decarbonation cycles. Formation of nano-inert metal oxides (CeO_2, $CaZrO_3$ and $Ce_{0.5}O_{0.5}O_2$) on CaO surface effectively mitigates the sintering in high-temperature carbonation/decarbonation by blocking the direct contact between the CaO nano-particles. The stability and enhanced reaction kinetics of the mixed oxide acceptors are due to high Tammann temperature and oxygen vacancies present in the inert dopent metal oxides, respectively.

Publications:

1. K. S. Sultana, S.A. Fagerbekk, T. Zhao, D. Chen: *Rational design of calcium based CO2 acceptors of different compositions with enhanced properties*. in preparation.
2. K. S. Sultana, D. Chen, *Enhanced hydrogen production by in-situ CO2 removal on CaCeZrOx nanocrystals*. Catalysis Today, 171(1) (2011) 43-51.

3. K. S. Sultanaa, Trung D.Tran, John C. Walmsley, Magnus Rønning, D. Chen: *CO2 capture on core-shell CaO/CaZrO3 composite with enhanced stability.* in preparation.

Sorption Enhanced Steam Reforming (SESR) process: an efficient route from biomass derived compounds to hydrogen production

Postdoctoral Fellow: Dr. Javier Fermoso

Supervisor: Prof. De Chen

Hydrogen is considered as a possible clean and environmentally friendly energy carrier for a sustainable energy system. Thus, a special attention is been paid to hydrogen production technology due to its increasing demand, not only in conventional industrial use (oil refining and synthesis of chemicals), but also the clean and efficient energy generation by means of the fuel cells. It requires H_2 production on a massive scale for transportation fuel production and stationary power generation. So, there is a crucial interest in developing new technologies to produce hydrogen from renewable sources, such as biomass, at high energy efficiency, cost attractive and in an environmental friendly manner. Recently, there has been growing interest in the called Sorption Enhanced Steam Reforming (SESR) process for hydrogen generation. The idea behind this novel reforming process is that steam reforming (SR), water gas shift (WGS) and CO_2 removal reactions occurs alongside in one reactor with a mixture of reforming catalyst and CO_2 acceptor. One important advantage of this process is that many types of biomass feedstock; from gas phase (biogas and syngas from biomass gasification), liquid phase (bioethanol, glycerol, bio-oils, etc.) to solid phase (raw lignocellulosic biomass) materials can be directly converted to high purity H_2 (>99 vol.%) without CO_2 emissions in a single reactor. In addition, new sorbents based on Ca are being developed which has shown improved CO_2 capture capacity, stability with respect to those obtained with naturally found materials, like artic dolomite, during the SESR process.

Publications and presentations

1. D. Chen, L. He. *Towards an efficient hydrogen production from biomass: a review of processes and materials*. ChemCatChem **3**, (2011) 490-511.
2. J. Fermoso, F. Rubiera, D. Chen. *Sorption enhanced catalytic steam gasification process: A direct route from lignocellulosic biomass to high purity hydrogen*. Energy Environ. Sci. **5** (2012) 6358-6367.
3. J. Fermoso, L. He, D. Chen. *Production of high purity hydrogen by sorption enhanced steam reforming of crude glycerol*. Int J Hydrogen Energy (Submitted).
4. J. Fermoso, L. He, D. Chen. *Sorption enhanced steam reforming (SESR): a*

direct route towards efficient hydrogen production from biomass-derived compounds. J. Chem. Technol. Biotechnol. (Submitted).
5. J. Fermoso, D. Chen. *High purity hydrogen production by sorption enhanced steam reforming of crude glycerol*. EuropaCat X**,** Catalysis – across the diciplines, 28 August – 02 September 2011, Glasgow, Scotland.

Engineering of Pt-based 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 various shape and composition 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 Pt surface structure and composition on the dehydrogenation reactions.

The project is aimed in that it 1) explores the novel Pt based nanoparticles with well controlled shapes, sizes and core-shell structures 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, 1) 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. 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. According to the experimental results, the catalytic performance indicates a strong structure-sensitive character. The reaction mechanism changes with the changing of the different ratio of Pt facets, {111} and {100}, edges and corners exposed on the catalyst surface. DFT simulation data are used to interpret the exprimental data and build up dehydrogenation kinetic model. 2) Various core-shell particles, such as Ru@Pt, Ir@Pt, Pd@Pt, Rh@Pt, Ag@Pt, and Co@Pt, have been synthesized and characterized by HRTEM, EDX-line scans, CO-stripping. Different core metals changes the binding energy of propane and hydrogen, so that changes the activity and selectivity of Pt catalysts in DHP.

Publications and presentations in 2011:

1. Jun Zhu, De Chen, Anders Holmen. *Carbon Nanofiber/Graphite Felt (CNF/GF) Composite for Waster Water and Crude Oil Purification*. Oral presentation. Carbon2011, Shanghai, July 24-29, 2011.
2. Jun Zhu, Minglei Yang, Yian Zhu, De Chen, Yingda Yu, Xinggui Zhou, Anders Holmen. *Selective C-H and C-C bond activation of propane on platinum nanoparticles with different sizes and shapes*. Oral presentation. EuropaCat X**,** Catalysis – across the diciplines, Glasgow, Scotland, 28 August – 02 September 2011
3. Jun Zhu, De Chen, Anders Holmen. *Selective C-H and C-C Bond Activation of Propane on Platinum Nanoparticles with Different Sizes and Shapes*. Oral presentation. Norwegian Catalysis Symposium 2011, Lillestrøm, September 28-29, 2011

Financial support:
The Norwegian Research Council (NFR).

Platinum based Catalysts for Methanol Fuel Cells: Metal Clusters and Carbon Supports

PhD candidate: Navaneethan Muthuswamy
Supervisors: Porf. De Chen, Prof. Mangnus Rønning

The project has dealt with synthesis and characterisation of advanced core-shell structurs for use as electrocatalysts for oxidation of small organic molecules, relevant for their direct electrochemical combustion in fuel cells.

The project has focused on two ultimate goals: the first is to reduce the Pt loading thereby reducing the cost and another is to tune the surface property of Pt, thereby enhancing the activity of MOR. Former is achieved by reducing Pt cluster size thus increase the Pt surface area, or by using Ru@Pt core-shell structure to reduce the Pt laoding but achieve similar Pt surface area. The surface property of Pt is tuned through Pt-graphite edge interface and by tailoring the RuPt architect in the shell of Ru@Pt core-shell NCs.

To achieve above goals, a proper synthesis method, ex-situ polyol method was adopted. In this method, monometallic Pt cluster size as well as Ru@Pt cluster size are controlled in colloid before depositing on corresponding supports. Results revealed the Pt dispersion was highly dependent on the amount of surface oxygen groups.

Methanol oxidation reaction was investigated on Pt clusters with various sizes on carbon nanofibers and carbon black supports with different surface oxygen concentration, aiming at gaining a better understanding of the relationship between the catalyst properties and the electrochemical

performance. It was found that CNF supported Pt clusters had better performance than carbon black supported Pt clusters for all the Pt particle sizes. Further, Pt supported on oxygen depleted CNF has better performance than the Pt supported on oxygen rich CNF. Owing to the combined advantages of optimum Pt particle size, oxygen free surface and unique properties of CNF, Pt supported on heat treated CNF exhibited a higher mass activity of about 2 times than the commercial E-TEK catalyst.

As another part of the advantage of ex-situ polyol method, RuPt shell architectures in the Ru@Pt cores-shell NCs were tailored by just controlling the pH of the synthesis medium during Pt deposition. Methanol oxidation reaction was investigated on carbon black supported Ru@Pt catalysts with different shell compositions. It was shown that the core-shell catalysts gave the highest steady-state current for methanol oxidation by a factor of 10 for alloyed shell and by a factor of 5 for Pt-enriched shell compared to the pure Pt catalyst. It can be concluded that the better catalytic performance of core-shell catalysts can be attributed to the ligand effect in the Pt enriched shell and a combination of ligand and bi-functional character in the alloyed shell.

Publications

1. Navaneethan Muthuswamy, Jose Luis Gomez de la Fuente, De Chen, Magnus Rønning, Svein Sunde, Piotr Ochal, Rajiv Giri, Steinar Raaen*: Towards highly efficient fuel cell catalyst: Optimization of particle size, supports and surface oxygen group concentration*. In Preparation.
2. Navaneethan Muthuswamy, Jose Luis Gomez de la Fuente, Trung Tran, De Chen, Magnus Rønning, Svein Sunde, John Walmsley, Piotr Ochal, Mikhail Tsypkin, Steinar Raaen: *RuPt nanoclusters for methanol oxidation: Effect of pH on the Ru encapsulation by Pt*. *In Preparation*
3. Piotr Ochal , Jose Luis Gomez de la Fuente, Mikhail Tsypkin, Frode Seland, Svein Sunde, Navaneethan Muthuswamy, Magnus Ronning, De Chen, Sergio Garcia, Selim Alayoglu, Bryan Eichhorn*: CO stripping as an electrochemical tool for characterization of Ru@Pt core-shell catalysts*. J. Electroanalytical Chemistry 655 (2011)140–146.

Advanced Catalysis in Methane Decomposition

Candidate: Fengliu Lou
Supervisor: De Chen

There is vast amount of methane in natural gas, so the efficient use is critical important. Carbon nanotube/nanofiber is a kind of novel nanomaterials with huge specific surface area, high electrical conductivity, and good chemical and thermal stability. In this project, carbon nanotube/nanofiber with controlled structure and CO-free hydrogen are produced by catalytic decomposition of

methane. Aligned carbon nanotubes that each nanotube has same orientation and length are synthesized over the surface of conductive substrate and clays for energy storage and mass production, respectively. Carbon nanofiber pellets are also obtained by using expended graphite as catalyst support, which could be used as catalyst support and electrode material. A fundamental study about the growth mechanism of carbon nanofiber will be investigated by using microkinetic model.

The objectives of this project is to obtain aligned carbon nanotubes on the surface of conductive substrates, clays and graphene, to prepare carbon nanofiber pellets with good mechanical strength and high surface area and to obtain a microkinetic model that can describe the carbon nanofiber/nanotube formation process.

Publications and presentations:

1. Fan Huang, Lou Fengliu, and Chen De: *Exploring Full Potential of ACNT@polyaniline arrays on Household Al as Highly Flexible and Cost-Effective Supercapacitors*. ChemSusChem, in press.
2. Fengliu Lou, Haitao Zhou, Fan Huang, Fride Vullum, De Chen: *Synthesis of MnO_2/Aligned Carbon Nanotubes/Aluminum Foil 3D Nanomaterials as Binder Free Cathode for High Performance Lithium Ion Battery*. in preparation.
3 Fengliu Lou, Fan Huang, Yingda Yu, and De Chen: *Synthesis of Carbon Nanofiber/Graphene Nanosheet Hybrids for Energy Storage*. in preparation.
4. Fengliu Lou, Haitao Zhou, Fan Huang, Fride Vullum, De Chen, Synthesis of MnO_2/Carbon nanofibers/Copper Foil 3D Nanomaterials as Binder Free Anode for High Performance Lithium Ion Battery. in preparation.
5. Fengliu Lou, Fan Huang, Estelle Vanhaecke, De Chen: *Synthesis of Carbon Nanotube Arrays on Metal Foils*. Poster presentation 2011 Annual World Conference on Carbon, Shanghai China,.
6. Fan Huang, Estelle Vanhaecke, Fengliu Lou, Edel Sheridan and De Chen: Synthesis and Applications of Core-Shelled Nanotube Arrays for Energy Storage. Oral presentation. 2011 Annual World Conference on Carbon, Shanghai China,

Financial support
The Norwegian Academy of Science and Letters (VISTA) Project: 6454

SINTEF projects

Catalytic hydrotreatment (HT) of bio-oils towards alkanes

Staff: SINTEF Materials and Chemistry, Dept. Process Chemistry: Senior scientist Rune Lødeng, Scientist Håkon Bergem, Chief Scientist Michael W. Stöcker, Scientist Lenka Hannevold.
NTNU, Dept. Chemical Engineering: Post. Doc. Sara B. Eiras, Professor Edd A. Blekkan

Project goals:
1) Oxygen removal; Establish fundamental knowledge on hydrodeoxygenation (HDO) and hydrogenation reactions of bio-oils from lignocellulose (bottle-necks and solutions), as basis for outlining practical processes from source to compatible fuel qualities
2) Identify catalyst materials with promising properties and to tune and optimize these for mild HDO of bio-oils
3) Develop new catalytic materials with properties suitable for deep HDO
4) Control of reaction selectivity (on a functional group level). Kinetics (activity and mechanisms) and stability will be addressed, and related to the properties of the feed
5) Obtain in-depth understanding of deactivation mechanisms and catalyst stability

Activities
Catalyst preparation and synthesis, characterization and testing
Hydrotreatment (HDO); Real bio oils and model components (phenol, guaiacol, benzofuran); Mini pilot test HDO rig with a fixed-bed continuous reactor.
Preparing for parallel testing in a 600 ml Parr Batch reactor in 2012.

Funding (2011 – 2012): The Norwegian Research Council

Refinery operations / Octane processes

Staff: Senior scientist Torbjørn Gjervan, Research scientist Hilde Bjørkan and Engineer Marianne Aune

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.

Client: Statoil R&D

Dehydrogenation of propane over chromium oxide based catalysts

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

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

Fischer-Tropsch catalysts

Staff: Research Scientist Rune Myrstad: 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 2011:
Ø. Borg, N. Hammer, B. C. Enger, R. Myrstad, O. A. Lindvåg, S. Eri, T. H. Skagseth, E. Rytter, *Effect of biomass-derived synthesis gas impurity elements on cobalt Fischer–Tropsch catalyst performance including in situ sulphur and nitrogen addition*, J. Catal. 279 (2011)

Client: Statoil R&D and The Research Council of Norway through the InGAP program

Microstructured Reactors for Compact Conversion of Natural Gas to Liquid Fuels

Staff: Research Scientist Rune Myrstad: SINTEF, Prof. Hilde Johnsen Venvik: NTNU

The objectives of this project are is increased knowledge on microstructured reactor technology for production of liquid fuels from natural gas:
- Fundamental knowledge on hybrid catalyst systems for direct synthesis of DME from synthesis gas in microstructured reactors
- Increased knowledge on the Co-catalyst in microstructured reactors and scale-up issues for a Fischer-Tropsch process

Publications and presentations in 2011:
F. Hayer, H. Bakhtiary-D., R. Myrstad, A. Holmen, P. Pfeifer, H. J. Venvik. *Synthesis of Dimethyl Ether from Syngas in a Microchannel Reactor - Simulation and Experimental Study*, Chem. Eng. J. 167 (2-3) (2011) 610

F. Hayer, H. Bakhtiary-D., R. Myrstad, A. Holmen, P. Pfeifer, H. J. Venvik. *Modeling and Simulation of an Integrated Micro Packed Bed Reactor-Heat Exchanger Configuration for Direct Dimethyl Ether Synthesis.",* Topics in Catalysis, 54 (13-15) (2011) 817

R.Myrstad. *Scale-up of microchannel reactors for small scale GTL processes*". Presented at 2nd Trondheim Gas Technology Conference, Trondheim, Norway, November 2-3, 2011

Client: The Research Council of Norway through the GASSMAKS program

CO_2 to dimethylether

Staff: Research Scientist Rune Myrstad: SINTEF

The goal of this project is to develop catalysts optimized for the hydrogenation of carbon dioxide to methanol/dimethylether under optimal membrane performance process conditions for the selective removal of water.

Client: EU FP7 (The CARENA project)

Cleaning of producer gas from biomass

Staff: Research Scientist Svatopluk Chytil: SINTEF and Prof. Edd Blekkan: NTNU

This project is a part of the KMB Biomass to Liquid Fuels (BTL), and the aim is to prepare Mn_xO_y-Al_2O_3 sorbents for H_2S removal from the producer gas from biomass gasification gas (producer gas).The main components of the producer gas are H2, CO, CO2, CH4, C2's, H2O, N2. However, the producer gas also contains pollutants/ contaminants that need to be removed prior to further downstream utilization. The relative concentration of the components in the producer gas depends on biomass source, gasifying agent, gasifier used and conditions employed.

Client: Statoil R&D and The Research Council of Norway through the Renergi program

Philosophiae Doctor (PhD) theses in 2011

Xuyen Kim Phan: *Catalysts formulations for use in microstructured reactors for conversion of synthesis gas to liquids.* Doctoral theses at NTNU, 2011:15

Fatemeh Hayer: *Direct Synthesis of Dimethyl Ether in Microstructured Reactors.* Doctoral theses at NTNU, 2011:81

Shreyas Panduran Rane: *Relation Between Catalyst Properties and Selectivity in Fischer-Tropsch Synthesis.* Doctoral theses at NTNU, 2011:156

Fan Huang: *3D Carbon/polyaniline Nanostructures for Energy Storage.* Doctoral theses at NTNU, 2011:215

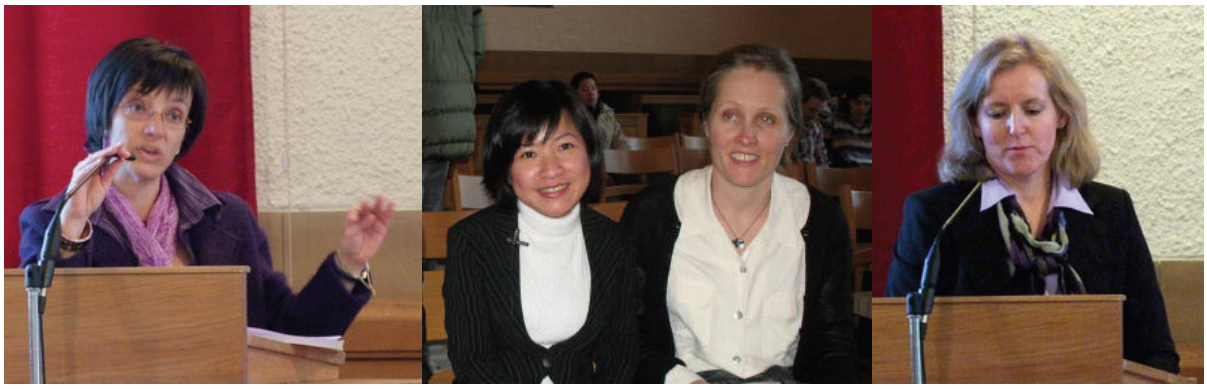
Oana Mihai: *Partial Oxidation of Methane by Chemical Looping.* Doctoral theses at NTNU, 2011: 232

Jia Yang: *A steady-State Isotopic Transient Kinetic Study of Cabalt Catalysts: Mechanistic Insights and Effect of Cabalt Particle Size, Supports and Promoters.* Doctoral theses at NTNU, 2011:280

Nikolaos E. Tsakoumis: *Deactivation of cobalt based Fischer-Tropsch synthesis catalysts.* Doctoral theses at NTNU, 2011:304

Kazi Saima Sultana: *Calcium Based CO_2 Acceptors for Sorption Enhanced Steam Methane Reformin. Doctoral thesis at NTNU. 2011:317*

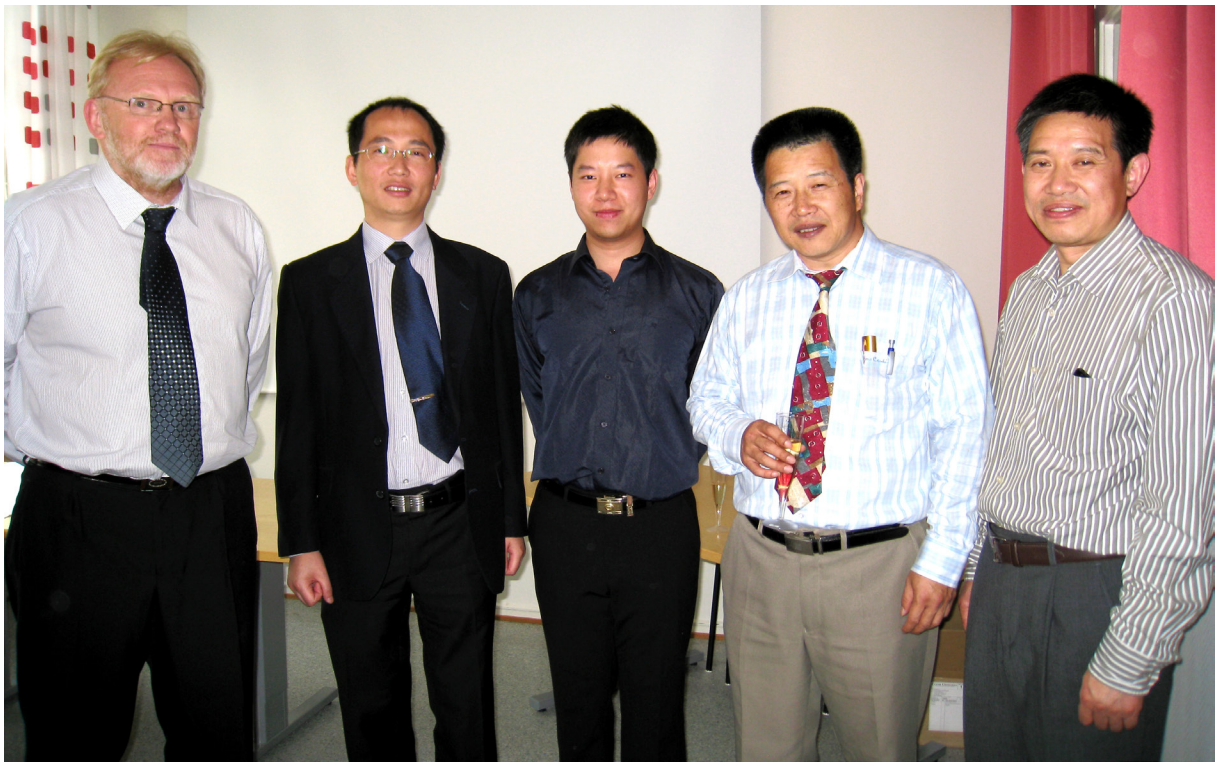
Navaneethan Muthuswany: *Platinum based Catalysts for Methanol Fuel Cells: Metal Clusters and Carbon Supports.* Doctoral theses at NTNU, 2011:335.



Disputas Xuyen Kim Phan 14/2011. From left: Prof. Stefania Specchia, Politecnico di Torino, Italy (opponent), Dr. Xuyen Kim Phan, Prof. Hilde Venvik (co-supervisor), Senior researcher Elisabeth Tangstad, SINTEF Oslo (opponent). Prof. Anders Holmen (supervisor), not shown.

Disputas Fatemeh Hayer 15/3-2011. From left: Dr. Margrete H. Wesenberg, Statoil (opponent), Prof. Edd A. Blekkan (administrator), Dr. Fatemeh Hayer, Prof. Jordi Llorca, Technical University of Catalonia, Spain (opponent), Prof. Hilde J. Venvik (supervisor), Prof. Anders Holmen (co-supervisor).

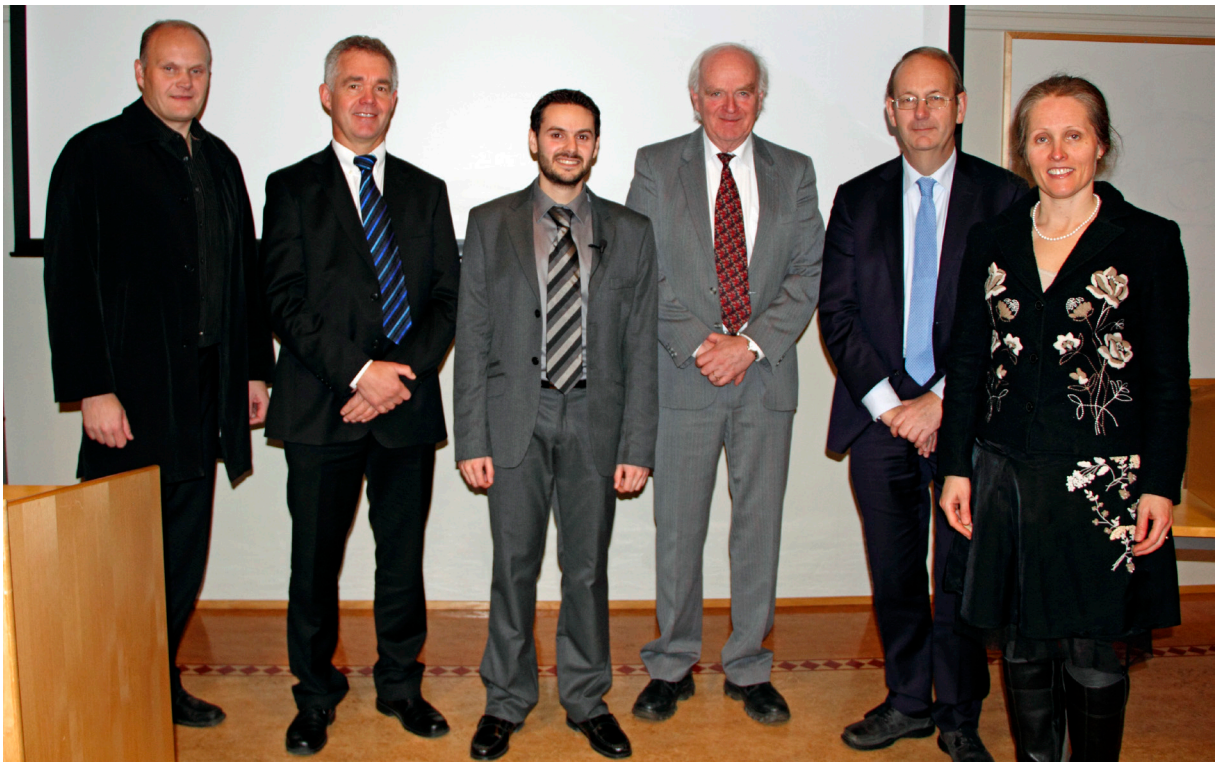
Disputas Shreyas Rane 20/5-2011. From left: Prof. Anja Olafsen Sjåstad, UiO (opponent), Dr. Shreyas Rane, Prof. Augustín Martínez, Institute of Catalysis and Petrochemistry, Valencia, Spain (opponent), Prof. Anders Holmen (supervisor). Prof. Erling Rytter and dr. Øyvind Borg, Statoil (co-supervisor) not shown.



Disputas Fan Huang 24/8-2011. From left: Prof. Edd Blekkan (administrator), Dr. Zhixin Yu, Statoil (opponent), Dr. Fan Huang, Prof. George Zheng Chen, University of Nottingham, UK (opponent), Prof. De Chen (supervisor).

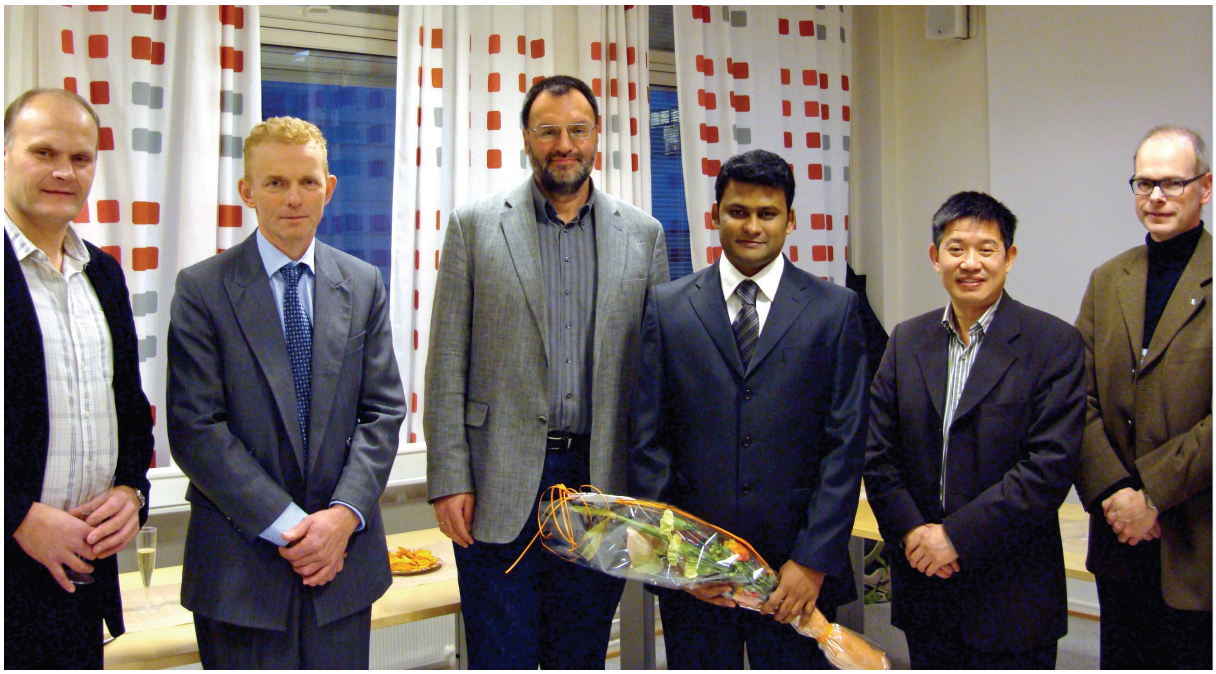
Disputas Oana Mihai 7/9-2011. From left to right: Prof. Klaus Jens, Telemark University College (opponent), Prof. Joris Thybaut, Ghent University, Belgium (opponent), Dr. Oana Mihai. Prof. Anders Holmen (supervisor) and Prof. De Chen (co-supervisor) not shown.

Disputas Jia Yang 28/8-2011. From left: Prof. Anders Holmen (supervisor), Prof. Edd A. Blekkan (administrator), Prof. Claude Mirodatos, IRCELYON-CNRS, France (opponent), Dr. Jia Yang, Prof. Unni Olsbye, UiO (opponent), Prof. De Chen, (co-supervisor).



Disputas Nikolaos Tsakoumis 18/11-2011. From left: Prof. Magnus Rønning (co-supervisor), Dr. Dag Schanke, Statoil (opponent), Dr. Nikolaos Tsakoumis, Prof. Anders Holmen, (supervisor), Prof. J.W (Hans) Niemantsverdriet, Eindhoven University of Technology, The Netherlands (opponent), Prof. Hilde J. Venvik (admimistrator). Prof. Erling Rytter and Dr. Øyvind Borg, Statoil (co-supervisors) not shown.

Disputas Saima Sultana Kazi 23/11-2011. From left: Prof. De Chen (supervisor), Prof. Anders Holmen (administrator), Prof. Øyvind Gregersen (Department head), Dr. Saima Sultana Kazi, Dr. Richard Blom, SINTEF Oslo (opponent), Prof. Johannes Hendrik (Harry) Bitter, Utrecht University, The Netherlands (opponent).



Disputas Navaneethan Muthuswamy 9/12-2011. From left: Prof. Magnus Rønning (administrator), Dr. Dag Øvrebø, Nordic power systems (opponent), Prof. Dr. Martin Muhler, Ruhr-University Bochum, Germany (opponent), Dr. Navaneethan Muthuswamy, Prof. De Chen (supervisor), Prof. Svein Sunde (co-supervisor).

Master (Diploma) Students in 2011

Mahmud Alam: *Kinetics and Deactivation in the Methanol Synthesis*

Claire Barilleau*: Conversion of synthesis gas from biomass to liquid fuels on promoted iron Fischer-Tropsch catalysts*

Ayob Esmaelpour*: Bifunctional catalyst for direct DME synthesis*

Aina Elin Karlsen*: Synthesis and Characterization of Co-based Fischer-TropschCatalysts and Supports, using hydrothermal and chemical attrition methods*

Ida Lien Bjørnstad*: Fotokatalytisk drivstoffproduksjon gjennom fotoreforming av hydrokarboner*

Loc Huu Nguyen*: Synthesis and Application of Nanomaterials in Clean Energy*

Kimete Osmani: *Water purification by using structured catalysts for hydrogenation of nitrates*

Katrine S. Biesterfeldt Plünnecke*: Catalytic Reforming of Producer Gas from Biomass Gasification.*

Damien Vannier*: Kinetic study of high temperature water gas shift reaction*

Group meetings with seminars
Spring 2011

Schedule	Time	Presenter	Topic
Jan 21	1300	Ilya V. Gorelkin	Concepts and models of the catalytic dehydrogenation of propane.
Feb 4	1300	Paul Radstake	Oxidative dehydrogenation of ethane over Pt-Sn catalysts.
Feb 18	1300	Hassan Jamil Dar	Simulation of Oxidative Dehydrogenation of Ethane to Ethylene in gas phase
Mar 2	1300	Dr. Elin Larsson, Insplorion AB	Nanoplasmonic sensing – applications for catalysis, hydrogen storage, polymers, corrosion and nanomaterials.
Mar 18	1300	Estelle Vanhaecke	Carbon nanostructured samples
Apr 1	1300	Alexey Voronov:	In situ study of the rhenium behaviour in Co-Re Fischer-Tropsch catalysts
Apr 29	1000	Saima S. Kazi	Development of new calcium-based CO_2 acceptors for steam methane reforming
May 6	1300	Eleni Patanou	Microcalorimetry.
May 13	1300	Cristian Ledesma Rodríguez	Hydrogen production by DME steam reforming over catalytic monoliths
June 10		Cancelled	
June 24	1300	Fan Huang	In-situ polymerization of polyaniline on CNT for supercapacitors

Fall 2011

Schedule	Time	Presenter	Topic
Aug 26	1300	Anna Lind, SINTEF	Supported iridium electrocatalysts for oxygen evolution in PEM electrolysers
Sept 9	1300	Ingeborg-Helene Svenum	Adsorbate induced segregation in a PdAg membrane model system: $Pd_3Ag(111)$
Sept 23	1300	Kumar Ranjan Rout	Modelling and Validation of Sorption Enhanced Steam Methane Reforming
Oct 7	1300	Dung Trung Tran, IFY	TEM characterization of catalytic materials
Oct 21	1300	Kay Gastinger, Søren Heinze	NTNU NanoLab Nanotechnology “hands on” - open for everyone
Nov 11	1300	Andrei Volynkin	Carbon as catalyst support in propane dehydrogenation
Nov 24	1000	Prof. Harry Bitter, Utrecht University, The Netherlands	Nanostructured carbon in catalysis – A Janus material
Dec 9	1300	Daham Gunawarda	Cancelled

Courses given by Group Members

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

TKP4150 Petrochemistry and oil refining

Responsible: Professor Edd A. Blekkan
Lecturers: Prof. Edd A. Blekkan, Adjunct Prof. Kjell Moljord (Statoil), Prof. Hilde Venvik, Prof. 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

TKP4190 - Fabrication and Applications of Nanomaterials

Responsible: Associate Professor Jens-Petter Andreassen
Lecturers: Prof. Hilde Venvik, Prof. Wilhelm Robert Glomm

Semester: Spring
Level: 3/4th year.
Credits: 7.5 SP
Restricted Admission: No
Course Plan: 3 Lectures, 2 hours exercises and 7 hours self study and assignments per week.

Objective:
To provide an overview of how nanoparticles can be made and applied within chemical processes

Prerequisites:
Basis chemistry and mathematics and course TMT4320 Nanomaterials.

Contents:
The thermodynamic driving force and the kinetics of nucleation and growth of nanoparticles is derived, focusing on precipitation from solutions. Different mechanism for nucleation and crystal growth along with calculations of nucleation and growth rates define the basis for design of different particle populations and applications relevant to research and industry.

The unique optical properties of nanoparticles made of noble metals such as gold and silver (localized surface plasmon resonance, LSPR), and how these can be implemented in detection and diagnostic applications via molecular spectroscopy. Use of nanomaterials such as gold nanoparticles, dendrimers, carbon nanotubes and plant viruses for medical applications such as chemotherapy and gene therapy.

Methods for the fabrication of catalysts and catalyst supports based on precipitation, along with other methods with particular relevance for the catalyst nanostructure and functionality, such as sol-gel and colloid based fabrication. Relevant examples where the significance of particle and pore size has been shown are included (Au, Co, Ni- catalysts and carbon nano fibres (CNF)). A short introduction to catalytic model systems and surface science and their experimental and theoretical application within nanocatalysis.

Teaching:
The course is given as a combination of lectures, compulsory exercises, laboratory demonstrations and project work with student presentations.

TKP4190 - Fabrication and Applications of Nanomaterials

Responsible: Professor Helge Weman, Department of Electronics and Telecommunications

Lecturers: Prof. Helge Weman, Prof. Thomas Tybell, Prof. Hilde Venvik, Prof. P. T. Sikorski, Assoc. Prof. R. Nydal

Semester: Fall
Level: 1st year.
Credits: 7.5 SP
Restricted Admission: No
Course Plan: 4 Lectures, 4 hours exercises per week.

Objective:
The subject gives an introduction to central themes within nanotechnology, with emphasis on how this cross-disciplinary technology can increase understanding and promote novel products.

Prerequisites: None

Contents:
The course presents an analysis of areas of relevance to subjects such as bionanotechnology, nanostructured materials, and nanoelectronics. The course will focus on common techniques in order to understand the possibilities of nanotechnology. A section on ethical, energy and environmental issues is also presented.

Teaching:
Lectures, mandatory exercises, laboratory demonstrations and group work. A continuous evaluation based on the exercises and group works will be used, each will be graded in percent.

Catalysis and petrochemistry MSc specialization

Coordinator: Professor Anders Holmen

Course description:

The specialization involves the following modules:

TKP4510 - Catalysis and Petrochemistry, Specialization Project	15 SP
TKP4515 - Catalysis and Petrochemistry, Specialization Course	7.5 SP
Module 1 (KAT) Heterogeneous catalysis. Advanced course	3.75 SP
Module 2 (KEM) Energy and environmental catalysis	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.

TKP4515-1 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:
Englis

KP4515-2 Environmental and energy catalysis

Responsible: 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 NOX, sulfur etc., but also for the development of selective processes. The course will give the fundamentals for catalytic processes for purification of exhaust gases (NOX, CO, unburned hydrocarbons etc). Within energy production the focus is on biofuel production, catalytic combustion, production of H2 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

KP8132 Applied heterogeneous catalysis

Responsible: Professor De Chen
Lecturers: Prof. Hilde J. Venvik and Prof. Anders Holmen

Credits: 7.5 SP
Prerequisites: TKP4155 Reaction kinetics and catalysis.

Course description:
The course is given every second year, next time in the fall term 2013.
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.

KP8133 Characterization of heterogeneous catalysts

Responsible: Professor Magnus Rønning

Credits: 7.5 SP

Course description:
The course is given every second year, next time in fall term 2012.
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.

KP8136 - Modelling of Catalytic Reactions

Responsible: Professor De Chen

Credits: 7.5 SP
Prerequisites: TKP4155 Reaction kinetics and catalysis.

Course description:
The course is given every second year, next time in spring 2013.

The course gives an overview on the methods for building microkinetic model, collecting or theoretically estimating rate constant, and microkinetic simulation. Focus will also on the microkinetic analysis of reaction systems at the atomic level. A project work of microkinetic modeling of a selected reaction system will be included in the course.

Learning methods and activities:
Seminars + project

Course materials:
James A. Dumesic, Dale F. Rudd, Luis M. Aparicio, James E. Rekoske, Andres A. Trenino, The microkinetics of heterogeneous catalysis. ACS professional Reference Book, Washington, DC 1993.
Selected papers

KP8137 - Design and Preparation of Catalytic Materials

Responsible: Prof Hilde Johnsen Venvik
Lecturer: Professor Edd Blekkan

Credits: 7.5 SP

Course description:
The course is given every second year, next time spring 2013.
The course gives an overview of principles for design and preparation of catalytic materials. Synthesis methods for support materials as well as catalytically active phases will be described, e.g. (co-)precipitation, impregnation incl. incipient wetness and ion exchange, deposition-precipitation, sol-gel methods, different methods based on pyrolysis and chemical vapour deposition (CVD). The different steps in the preparation, including drying, calcination and reduction, and parameters that influence/control the final catalyst properties are assessed. Important classes of materials such as alumina, silica and zeolites, as well as structured mesoporous materials (MCM-41, SBA-15) are discussed. Carbon nanofiber (CNF) production by catalytic methods is also included, and an introduction to combinatorial methods for parallel synthesis and/or screening of new catalyst systems will be given. Methods for and challenges connected to synthesis scale-up and industrial processing of heterogeneous catalysts are specifically treated.

Learning objective:
The students should be able to make qualified choices and adjustments regarding catalyst preparation methods and synthesis parameters. To some extent they should be able to assess scale-up and industrial production.

Learning methods and activities:
Seminars

Recommended previous knowledge:
Basic knowledge in solid state chemistry and heterogeneous catalysis is required.

Course materials:
Selected handouts and scientific papers

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

Responsible: 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 2011

1. T. Zhao, I. Kvande, Y. Yu, M. Rønning, A. Holmen, D. Chen: Synthesis of platelet carbon nanofiber/carbon felt composite on in-situ generated Ni-Cu nanoparticles. J. Phys. Chem. C **115** (2011) 1123-1133.

2. O. Mihai, D. Chen, A. Holmen: Catalytic consequence of oxygen of lanthanum ferrite perovskite in chemical looping reforming of methane. Ind. Eng. Chem. Res. **50** (2011) 2613-2621.

3. H. Bakhtiary, F. Hayer, X.K. Phan, R. Myrstad, H.J. Venvik, P. Pfeifer, A. Holmen: Characteristics of an Integrated Micro Packed Bed Reactor-Heat Exchanger for Methanol Synthesis from Syngas. Chem. Eng. J. 167 (2011) 496-503.

4. F. Hayer, H. Bakhtiary, R. Myrstad, A. Holmen, P. Pfeifer, H. Venvik: Synthesis of dimethyl ether from syngas in a microchannel reactor - Simulation and experimental study. Chem. Eng. J. 167 (2011) 610-615.

5. D. Chen, R. Lødeng, H. Svendsen, A. Holmen: Hierarchical multiscale modelling of methane steam reforming reactions. Ind. Eng. Chem. Res. 50 (2011) 2600-2612.

6. S. Lögdberg, M. Boutonnet, J.C. Walmsley, S. Järås, A. Holmen, E.A. Blekkan: Effect of water on the space-time yield of different supported cobalt catalysts during Fischer-Tropsch synthesis. Appl. Catal. A: General 393 (2011) 109-121.

7. D. Chen, K. Moljord, A. Holmen: Methanol to Olefins: Coke Formation and Deactivation. In: Deactivation and Regeneration of Zeolite Catalysts, M. Guisnet, F.R. Ribero (Eds). Imperial College Press, London, 2011. ISBN 978-1-84816-6370. 269-292.

8. Bjørn Christian Enger, Åse-Lill Fossan, Øyvind Borg, Erling Rytter, Anders Holmen, Modified alumina as catalyst support for cobalt catalysts in the Fischer Tropsch synthesis. J. Catal. **284** (2011) 9-12

9. Roya Dehghan, Thomas W. Hansen, Jacob B. Wagner, Anders Holmen, Erling Rytter, Øyvind Borg, Johmn C. Walmsley: In situ Reduction of Promoted Cobalt Oxide Supported on Alumina by Environmental Transmission Electron Microscopy. Catal Lett. **141** (2011) 754-761

10. S. Boullosa_Eiras, E. Vanhaecke, T. Zhao, D. Chen, A. Holmen: Raman and X-ray investigations of the phase transformation of ZrO_2-Al_2O_3 and CeO_2-Al_2O_3 nanocomposites. Catal. Today **166** (2011) 10-17

11. Sara Boullosa-Eiras, Tiejun Zhao, De Chen, Anders Holmen: Effect of the preparation methods and alumina nanoparticles on the catalytic performance of $Rh/Zr_xCe_{1-x}O_2$-Al_2O_3 in methane partial oxidation. Catal. Today **171** (2011) 104-115

12. Sarka Zarubova, Shreyas Rane, Jia Yang, Yingda Yu, Ye Zhu, De Chen, Anders Holmen: Fischer-Tropsch synthesis on Hierarchically Structured Co-Nanoparticles/Carbon Nanofibers/Carbon-felt- Composites. ChemSusChem **4** (2011) 935-942.

13. Xuyen K. Phan, Jia Yang, Hamid Bakhtiary-Davijnay, Rune Myrstad, Hilde J. Venvik, Anders Holmen: Studies of Macroporous Structured Alumina Based Cobalt Catalysts for Fischer-Tropsch Synthesis. Catal. Lett. 141 (2011) 1739-1745.

14. Xuyen K Phan, Hamidreza Bakhtiary-Davijany , Rune Myrstad; Peter Pfeifer, Hilde J Venvik, Anders Holmen, Preparation and performance of Cu-based monoliths for methanol synthesis. Appl. Catal. A: General **405** (2011) 1-7

15. T. Zhao, S. Boullosa-Eiras, Y. Yu, D. Chen, A. Holmen, M. Rønning: Synthesis os supported catalysts by impregnation and calcination of low-temperature polymerizable metal-complexes. Top. Catal. **54** (2011) 1163-1174.

16. Hamid Bakhtiary Davijany, Fatemeh Hayer, Xuyen Kim Phan, Rune Myrstad, Peter Pfeifer, Hilde J. Venvik, Anders Holmen: Performance of a multi-slit packed bed microstructured reactor in the synthesis ofr methanol: Comparison with a laboratory fixed-bed reactor. Chem. Eng. Sci. **66** (2011) 6350-6357.

17. J.M. Gonzalez-Carballo, Jia Yang, A. Holmen , S. Garcia-Rodrigues, S. Rojas, M. Ojeda, J.L.G. Fierro: Catalytic effect of ruthenium particle size on the Fischer-Tropsch Synthesis.
J. Catal. **284** (2011) 102-108.

18. F. Hayer, H. Bakhtiary, R. Myrstad, A. Holmen, P. Pfeifer, H.J. Venvik: Modelling and Simulations of an Integrated Micro Packed Bed Reactor-Heat Exchanger Configuration for Direct Dimethyl Ether Synthesis. Top. Catal. **54** (2011) 817–827.

19. J.P. den Breejen, A.M. Frey, J. Yang, A. Holmen, M.M. van Schooneveld, FM.F. de Groot, O. Stephan, J.H. Bitter, K.P. de Jong: A Highly Active and Selective Manganese Oxide Oxide Promoted Cobalt-on-Silica Fischer-Tropsch Catalyst. Top. Catal. **54** (2011) 768–777.

20. R. Lødeng, E. Bjørgum, B.C. Enger, J.L. Eilertsen, A. Holmen, B. Krogh, I. Aartun Bøe, M. Rønnekleiv, E. Rytter: A Fixed-Bed Reactor Study of Catalytic Partial Oxidation over Rh/Al_2O_3: An Indication of a Direct Pathway to CO. Top. Catal. **54** (2011) 873–880.

21. E. Vanhaecke, F. Huang, Y. Yu, M. Rønning, A. Holmen, D. Chen: Catalytic Consequence of the Interface Between Iron Catalysts and Foils in Synthesis of Aligned Nanocarbons on Foils. Topics Catal. **54** (2011) 986–997.

22. S. Boullosa Eiras, T. Zhao, E. Vanhaecke, D. Chen, A. Holmen: Partial Oxidation of methane to synthesis gas on $Rh/Zr_xCe_{1-x}O_2$-Al_2O_3. Catal. Today **178** (2011) 12-24.

23. D Chen, Li He: Towards an Efficient Hydrogen Production from Biomass: A Review of Processes and Materials. ChemCatChem 3(3) (2011) 490-511

24. D. Chen, Chang-Jun Liu: A Current Perspective on Catalysis for New Energy Technologies. *ChemCatChem* 3(3) (2011) 423-425

25. C. Fan, Xing-Gui Zhou, De Chen, H.Y. Cheng, Yi-An Zhu: *Toward CH4 dissociation and C diffusion during Ni/Fe-catalyzed carbon nanofiber growth: A density functional theory study*. J. Chem. Phys. (134) 2011

26. N. Hammer, K. Mathisen, Tina Zscherpe, De Chen, M.agnus Rønning: *Effect of Pretreatment on Carbon-Supported Au/TiO_2 Catalysts for Preferential Oxidation of CO*. Topics Catal. 54 (2011) 922-930

27. X.X. He, C. Fan, XY Gu, De Chen, Yi-An Zhu: *Role of CO2 in ethylbenzene dehydrogenation over Fe2O3(0001) from first principles*. J. Mol. Catal. A: Chemical 344(1-2) (2011) 53-61.

28. Saima Sultana Kazi, De Chen**:** *Enhanced hydrogen production by in situ CO2 removal on CaCeZrOx nanocrystals*. Catal. Today 171 2011 43-51

29. Qing Li, Zhijun Zhijun Sui, Xinggui Zhou, De Chen: *Kinetics of propane dehydrogenation over Pt-Sn/Al_2O_3 catalyst*. Appl. Catal. A : General 398 (2011) 18-26

30. Qing Li, Zhijun Sui, Xinggui Zhou, Yian Zhu, Zhou, Jinghong Zhou, De Chen: *Coke Formation on Pt-Sn/Al_2O_3 Catalyst in Propane Dehydrogenation: Coke Characterization and Kinetic Study*. Top. Catalysis 54 (2011) 888-896

31. Piotr Ochal, Jose Luis de la Fuente Gomez, Mikhail Tsypkin, Frode Seland, Svein Sunde, Navaneethan Muthuswamy, Magnus Rønning, De Chen, S. Garcia, Selim Alayoglu, Brian Eichhorn: *CO stripping as an electrochemical tool for characterization of Ru@Pt core-shell catalysts*. J. of Electroanal. Chem. 655(2) (2011) 140-146

32. Yuefa Wang, Zhongxi Chao, De Chen, Hugo Atle Jakobsen: *SE-SMR process performance in CFB reactors: Simulation of the CO2 adsorption/ desorption processes with CaO based sorbents.* Int.J. Greenhouse Gas Control 5(3) (2011) 489-497

33. ML. Yang, Yi-An Zhu, C. Fan, Zhi-Jun Sui, De Chen, Xing-Gui Zhou: *DFT study of propane dehydrogenation on Pt catalyst: effects of step sites.* Phys. Chem. Chem. Phy. (PCCP) 13(8) (2011) 3257-3267

34. Qi Zhou, Ping Li, XL Wang, Xing-Gui Zhou, Daijun Yang, De Chen: *Preparation of CNF-supported Pt catalysts for hydrogen evolution from decalin*. Materials Chem. Phys. 126(1-2) (2011) 41-45

35. Espen Standal Wangen, Amin Osatiashtiani, Edd A. Blekkan: *Reforming of syngas from biomass gasification: Deactivation by tar and potassium species.* Topics Catal. 54 (2011) 960-966.

36. M. Lualdi, S. Lögdberg, G. Carlo, S. Järås, M. Boutonnet, A.-M. Venezia, E.A. Blekkan, A. Holmen. *Evidence for Diffusion-Controlled Hydrocarbon Selectivities in the Fischer-Tropsch Synthesis Over Cobalt Supported on Ordered Mesoporous Silica.* Topics Catal. 54 (2011) 1175-1184.

37. E.A. Blekkan, De Chen, M. Rønning, H.J. Venvik: *Preface: Catalysis for Clean Energy.* Topics Catal. 54 (2011) 755-756.

Presentations at International and National Meetings in 2011

1. A. Voronov, N. E. Tsakoumis, Ø. Borg, E. Rytter, A. Holmen, M. Rønning, *Deactivation studies of Co-based Fischer-Tropsch catalysts by in-situ spectroscopies at realistic working conditions*. ESPCA School, January 17-25 2011, Campinas, Brazil.

2. S. Rane, A. Holmen*, J. Yang, B. C. Enger, E. Rytter: *Alumina Supported Co Catalysts for Fischer-Tropsch Synthesis. Effect of Particle Size and Alumina Modifications on Activity and Selectivity.* Lecture. 22st North American Catalysis Society Meeting, June 6 – 10 2011, Detroit, USA.

3. A.H. Lillebø, C. Balonek, S, Rane, B. Enger, E. Rytter, E.A. Blekkan, A. Holmen*: Effects of Li, Na, K and Ca on Co-based Fischer-Tropsch Catalysts*. Poster. EuropaCat X. August 28 – September 2011, Glasgow, Scotland.

4. B.C. Enger, V. Frøseth, E. Rytter, A. Holmen: *Effects of Zn during SSITKA studies of Co-Re/γ-Al_2O_3 catalyst in the Fischer-Tropsch synthesis.* Poster. EuropaCat X. August 28 – September 2011, Glasgow, Scotland.

5. J. Yang*, Ø. Borg, D. Chen, A. Holmen*: A study of chain termination and propagation on 20%Co/CNT Fischer-Tropsch catalyst*. Oral presentation. EuropaCat X. August 28 – September 2011, Glasgow, Scotland.

6. J. Zhu*, M. Yang, Y. Zhu, D. Chen, Y. Yu, X. Zhou, A. Holmen: *Selective C-H and C-C bond Activation of Propane on Platinum Nanoparticles with Different Sizes and Shapes.* Oral presentation. EuropaCat X. August 28 – September 2011, Glasgow, Scotland.

7. X.K. Phan, J. Walmsley, H. Bakhtiary-Davijany, R. Myrstad, P. Pfeifer, A. Holmen, H. Venvik: *Characterization and Performance of Pd/CeO_2 Catalysts as a Powder in Fixed-bed Reactor and as a Coating in a Stacked Foil Microreactor for Methanol Synthesis*. Poster. EuropaCat X. August 28 – September 2011, Glasgow, Scotland.

8. N.E. Tsakoumis, A. Voronov, M. Rønning. Ø. Borg, E. Rytter, A. Holmen: *An operando study of Co-based Fischer-Tropsch synthesis catalysts*. Poster. EuropaCat X. August 28 – September 2011, Glasgow, Scotland.

9. J.M. Gonzalez-Carballo, Jia Yang, S. Garcia, M. Ojeda, A. Holmen, J.L.G. Fierro, S. Rojas: *Ruthenium particle size effect on the Fischer-Tropsch*

Synthesis. Poster. EuropaCat X. August 28 – September 2011, Glasgow, Scotland.

10. T. Zhao*, M. Rønning, X. Zhou, D. Chen, A. Holmem, W. Yuan: *Towards understanding the graphene sheet orientation in carbon nanostructures by a diffusion-nucleation model*. 6th Asia Pacific Reaction Engineering Symposium (APCRE'11). September 18-21 2011, Bejing, China.

11. A. Holmen: *Alumina Supported Co Catalysts for Fischer-Tropsch Synthesis, Effect of Particle Size and Alumina Modifications on Activity and Selectivity.* Plenary Lecture. Norwegian Catalysis Symposium 2011. Landsmøte i Kjemi. September 28-29 2011, Norges Varemesse, Lillestrøm.

12. A. Lillebø, C. Balonek, S. Rane, E. Rytter, E.A. Blekkan, A.. Holmen*: Fischer-Tropsch biomass to liquids, effect of LI, Na, K, and Ca on Cobalt catalysts.* 1st International Congress on Catalysis for Biorefineries (CatBior 2011). October 2-5 2011. Malaga, Spain.

13. A. Holmen* and H. Venvik*: Microstructured reactors for production and conversion of synthesis gas*. Invited lecture. Colloquium on Chemical Reaction Engineering (CCRE-2011) on Methane Valorization. October 10-11 2011, Technical University Munich, Garching, Germany

14. A. Holmen: *Recent Developments in Direct Routes for Natural Gas Conversion.* Keynote Lecture. 2nd Trondheim Gas Technology Conference. November 2-3 2011, Trondheim, Norway.

15. R. Myrstad*, H. Baktiary-Davijany, H. Venvik, A. Holmen, P, Pfeiffer: *Scale-up microchannel reactors for small scale GTL processes.* Lecture. 2nd Trondheim Gas Technology Conference. November 2-3 2011, Trondheim, Norway.

16. E. Blekkan, S. Chytil, A.H. Lillebø, B.C. Enger, A. Holmen: *Biomass to liquid fuels - BTL.* Poster. 2nd Trondheim Gas Technology Conference. November 2-3 2011, Trondheim, Norway.

17. P.V.D.S. Gunawardana, J. Walmsley, T.T.M. Nguyen, E. Edwin, A. Holmen, D. Chen, H.J. Venvik: *Metal dusting corrosion initiation in conversion of natural gas to synthesis gas*. Poster. 2nd Trondheim Gas Technology Conference. November 2-3 2011, Trondheim, Norway.

18. De Chen*, Towards an efficient hydrogen production from biomass*. Oral presentation. 1st international symposium on chemistry for energy conversion and storage. 27 Feb.- 2 March, 2011, Berlin, Germany.
19. Fan Huang, Estelle Vanhaecke, De Chen: *ACNT@PANI composites for Energy Storage,* Poster. 1st international symposium on chemistry for energy conversion and storage. 27 Feb.- 2 March, 2011 Berlin, Germany.

20. Xinggu Zhou, De Chen, Weikang Yuan*, Structure-Directing Manipulation of Catalyst Surface for Better Kinetic Behaviors*. Plenary lecture. 6th Asia Pacific Chemical Reaction Engineering Symposium. September 18-21, 2011. Beijing, China.

21 Javier Fermoso Dominguez, Li He, De Chen*, Towards an efficient hydrogen production from biomass*, Keynote lecture. 6th Asia Pacific Chemical Reaction Engineering Symposium. September 18-21, 2011. Beijing, China.

22. X. Duan, J. Zhou, G. Qian, P. Li, X. Zhou, De Chen: *DFT study of Ammonia Decomposition on trasition metals*. Oral presentation. 6th Asia Pacific Chemical Reaction Engineering Symposium. September 18-21, 2011. Beijing, China.

23. Q. Li, Z. Sui, X. Zhou, D. Chen: *Kinetic study of propane dehydrogenation.* Oral presentation. 6th Asia Pacific Chemical Reaction Engineering Symposium. September 18-21, 2011. Beijing, China.

24. Jun Zhu, De Chen*, Anders Holmen, *Carbon Nanofiber/Graphite Felt (CNF/GF) Composite for Waster Water and Crude Oil Purification*. Oral presentation. Carbon conference, July 24-29, Shanghai, China.

25. Fengliu Lou, Fan Huang, Estelle Vanhaecke De Chen*: Synthesis of Carbon Nanotube Arrays on Metal Foils*. Poster presentation, Carbon conference, July 24-29, Shanghai China.

26. Fan Huang, Estelle Vanhaecke, Fengliu Lou, Edel Sheridan and De Chen: *Synthesis and Applications of Core-Shelled Nanotube Arrays for Energy Storage,* Oral presentation. Carbon conference, July 24-29, Shanghai, China.

27. De Chen: *3D engineering design of nano-structured composites for energy storage*. Oral presentation. The 3rd Global Chemical Engineers Seminar. July 16-19, 2010, Beijing, China.

28. Jun Zhou, Anders Holmen, De Chen: *Selective C-H and C-C bond activation of propane on platinum nanoparticles with different sizes and shapes*. Oral presentation. EuropaCat X 2011, Scotland, 29 August – 2 September, 2011.

29. J. Fermoso and D. Chen: *High purity hydrogen production by sorption enhanced steam reforming of crude glycerol*, Poster presentation. EuropaCat X 2011, Scotland, 29 August – 2 September 2011.

30. M. Surma, T. Fuglerud, C. Lamberti and De Chen: *Transient kinetic investigation of Ethylene Oxychlorination.* Poster presentation. EuropaCat X 2011, Scotland. 29 August – 2 September 2011.

31. Eleni Patano, De Chen, Edd Blekkan: Microcalorimetric studies of cobalt supported catalysts for Fischer-Tropsch synthesis. Poster presentation. EuropaCat 2011, Scotland. 29 August – 2 September 2011.

32. Jun Zhou, M. Surma, T. Fuglerud, C. Lamberti and De Chen. *Transient kinetic investigation of Ethylene Oxychlorination.* Oral presentation, InGap Seminar, Trondheim, Norway, December 1, 2011.

33. Hassan J. Dar, Sandro U. Nanot, Klaus. J. Jens, Hugo A. Jakobsen, Elisabeth Tangstad, De Chen: *Kinetic analysis of gas phase oxidative dehydrogenation for ethane to ethylene at atmospheric pressure*. Oral presentation. InGap Seminar, Trondheim, Norway, December 1 2011.

34. Jia Yang, De Chen, Anders Holmen: *A study of chain propagation and termination on a Fischer-Tropsch catalyst*. Oral presentation, Norwegian Symposium on Catalysis, 27 Sept., 2011, Lillestrom,.

35. Jun Zhou, Anders Holmen, De Chen*: Selective C-H and C-C bond activation of propane on platinum nanoparticles with different sizes and shapes*. Oral presentation. Norwegian Symposium on Catalysis, 27 Sept., 2011 Lillestrom.

36. De Chen: *Nanomaterials for energy storage*.Oral presebtation. Nanolab Seminar, NTNU, 25 Oct. 2011.

37. Espen Standal Wangen, Edd A. Blekkan: *Catalytic conditioning of bio-syngas*. GreenSyngas workshop. 23. February 2011, Güssing, Austria,.

38. I. V. Gorelkin, E.A. Blekkan: *Concepts and models of the catalytic dehydrogenation of propane.* 22nd North American Catalysis Society Meeting, June 5-10, 2011, Detroit, USA.

39. Edd A. Blekkan: *GTL - Gas to liquids - Biomass-to-liquids (BTL*). Bergen Gas Conference, May 4-5, 2011.

40. E. Patanou, De Chen, E.A. Blekkan. *Microcalorimetric studies on cobalt supported catalysts for Fischer – Tropsch synthesis*. Poster. EuropaCat X, Aug 28 – Sept 2, 2011Glasgow, Scotland.

41. E. Patanou, E.A. Blekkan: *Hydrogen adsorption on supported cobalt catalysts for the Fischer-Tropsch synthesis studied by microcalorimetry.* Norwegian Symposium on Catalysis, 27 Sept., 2011 Lillestrøm.

42. I. V. Gorelkin, E.A. Blekkan. *Concepts and models of the catalytic dehydrogenation of propane*. EuropaCat X, Aug 28 – Sept 2, 2011Glasgow, Scotland.

43. S. Chytil, A. Lind, A.H. Lillebø, B.C. Enger, A. Holmen, E.A. Blekkan. *Biomass to liquid fuels - BTL.* 2nd Trondheim Gas Technology Conference, Nov. 2-3, 2011, Trondheim

44. S. Chytil, A. Lind, E. Vanhaecke, E.A. Blekkan. *Preparation and characterization of MnxOy-Al2O3 sorbents for H2S removal from biomass gasification gas.* Poster. 2nd Trondheim Gas Technology Conference, Nov. 2-3, 2011, Trondheim

45. Ingeborg-Helene Svenum, Manos Mavrikakis, Hilde J. Venvik. *Adsorbate induced segregation in Pd3Ag(111).* Oral presenation. 10th International Conference on Catalysis in Membrane Reactors (ICCMR); June 20-24 2011.

Seminars 2011

Inauguration of Kjemihall D

Prolongation of Geminisenter: KinCat

Thursday June 16, 2011 at 10.15 – 13.-00

Program:

1015 Official opening by Prorektor Kari Melby

Jens Rostrup-Nielsen, Halldor Topsøe, Danmark: *Prospects for natural gas conversion.*

Erling Rytter, Statoil: *25 years of cooperation within hydrocarbon conversion – experiences and perspectives.*

Anders Holmen, NTNU: *Past and future use of Kjemihall D*

Poster presentations and lunch in Kjemihall D

The inauguration is open for all!

KinCat
Catalysis Group – SINTEF – NTNU

Seminar "Anders Holmen"

December 2, 2011, NTNU, Auditorium R8.

Program

08:30 Registration/coffee

09:00 De Chen: Opening/Welcome

09:10 Edd A. Blekkan, NTNU, Norway: *Anders Holmen: Highlights.*

09:30 Erling Rytter, Statoil and Steinar Kvisle, INEOS: *Anders Holmen: Industrial importance.*

10:00 Gabor Somorjai, Univ. of California, Berkeley, USA: *Revolution in Molecular Catalysis Science.*

10:45 Coffee break

11:15 Krijn P. de Jong, Utrecht Univ., The Netherlands: *Fundamental studies on the synthesis of supported metal catalysts.*

11:45 Lars J. Petterson, KTH, Stockholm, Sweden: *Putting chemical engineering in the driver´s seat: Catalytic solutions for solving emission and efficiency problems in the automotive sector for 2020 and beyond.*

12:15 Lunch

13:15 Claude Mirodatos, IRC Lyon, France: *Recent trends in natural and bio-gas conversion.*

13:45 Tapio Salmi, Åbo Akademi, Finland: *Challenges of reaction engineering in the shift towards renewables.*

14:15 Guy Marin, Univ. Gent, Belgium: *The quasi-steady state approximation in kinetics: application to some industrial reactions.*

14:45 Coffee/Fruit

15:15 Alessandra Beretta, Politecnico di Milano: *Short contact time CPO of light hydrocarbons investigated through advanced experimental and modelling tools.*

15:45 Unni Olsbye, Univ. of Oslo, Norway: *Back to basics: Kinetic significance of catalyst supports in methane to syngas processes.*

16:15 Anders Holmen, NTNU: *Concluding remarks.*

16:30 End of seminar

19:30 Dinner: Grenaderen Restaurant

Seminar “Anders Holmen”. From left: Magnus Rønning, Hilde J. Venvik, Alessandra Beretta, Gabor Somorjai , Unni Olsbye, Steinar Kvisle, Edd A. Blekkan, Anders Holmen, Tapio Salmi, Guy Marin, Lars Pettersson, Claude Mirodatos, De Chen

Alumni
PhD students Catalysis group:

Per Åge Sørum
Hydrogenolysis of esters. Conversion of metylformiat to methanol
Defense of thesis: 1982
Current position: Statoil Mongstad

Edd Anders Blekkan.
Characterization and pyrolysis of heavy oils.
Defense of thesis: November 1985
Current position: Professor NTNU.

Dag Schanke.
Hydrogenation of CO over supported iron catalysts.
Defense of thesis: October 1986
Current position: Chief researcher, Statoil

Kjell Moljord
Diffusion og reaksjon i sure organiske ionebyttere: Væskefase dehydratisering av metanol og t-butanol katalysert av sulfonert poly(styrene-divinylbenzen.
Defense of thesis: 1986
Current position: Statoil, Adjunct professor, NTNU

Edvard Bergene
Surface characterization of Pt and Pt/Rh gauze catalysts.
Defense of thesis: March 1990
Current position: Statoil

Rune Lødeng
Title of thesis: A kinetic model for methane directly to methanol.
Defense of thesis: 1991
Current position: Senior researcher,SINTEF Trondheim

Trude Dypvik
Oligomerization of ethene on zeolite ZSM-5 type catalysts
Defense of thesis: January 1992
Current position: Senior advisor, The Research Council of Norway

Ola Olsvik
Thermal coupling of methane
Defense of thesis: 1993
Current position: Statoil

Anne Hoff
CO hydrogenation over cobalt Fischer-Tropsch catalysts.
Defense of thesis: October 1993
Current position: Statoil

Stein Harald Skaare.
Reaction and heat transfer in wall-cooled fixed bed reactor
Defense of thesis: December 1993
Current position: Aibel, Oslo

Odd Arne Bariås
Transient kinetic investigation of the catalytic dehydrogenation of propane
Defense of thesis: December 1993
Current position: Elkem Solar AS

Geir Remo Fredriksen
Hydrogenation of CO on supported cobalt catalysts studied by in situ FTIR spectroscopy
Defense of thesis: December 1993
Current position: Statoil

Arne Grønvold
Conversion of methanol to lower alkenes over molecular sieve-type catalysts
Defense of thesis: September 1994
Current position: Ineos

Sturla Vada
Isotopic transient kinetic investigations of catalytic reactions.
Defense of thesis: October 1994
Current position: Statoil

Rune Prestvik
Characterization of the metal function of a Pt-Re/Al2O3 reforming catalyst.
Defense of thesis: October 1995
Current position: Statoil

Anne-Mette Hilmen
Reduction and reoxidation of cobalt Fischer-Tropsch catalysts
Defense of thesis: October 1996
Current position: Shell, Norway

Karina Heitnes Hofstad
Catatlytic oxidation of methane to synthesis gas
Defense of thesis: 1996
Current position: Statoil

Håkon Bergem
Sulfur toerant zeolite supported platinum catalysts for aromatics hydrogenation.
Defense of thesis: April 1997
Current position: Senior researcher, SINTEF

Staale Førre Jenssen
Catalytic decomposition of NO over metal exchanged zeolites
Defense of thesis: January 1998
Current position: Statoil

Mimmi Kjetså
Etherification of methanol and iso/n-propanol with C4–C6 olefins on a macroporous acid ion exchange resin catalyst
Defense of thesis: May 1998
Current position: Statoil

De Chen
Methanol conversion to light olefins over SAPO-34: Diffusion, coke depositions and shape selective reactions.
Defense of thesis: 1998
Current position: Professor, NTNU

Hans Petter Rebo
Application of the TEOM reactor for adsorption, diffusion and kinetic studies
Defense of thesis: March 1999
Current position: Statoil

Marit Senum Brownrigg
Deactivation and regeneration of bifunctional zeolites
Defense of thesis: August 1999
Current position: Jotun, Dubai.

Ketil Firing Hanssen
Cobalt Fischer-Tropsch catalysts studied by steady-state and transient kinetic methods
Defense of thesis: 1999
Current position: Senior engineer, Det norske veritas (DNV)

Magnus Rønning
Bimetallic catalysts and platinum surfaces studied by X-ray absorption spectroscopy and scanning tunnelling microscopy.
Defense of thesis: February 2000
Current position: Professor, NTNU

Marcus Fathi
Catalytic partial oxidation of methane to synthesis gas.
Defense of thesis: September 2000
Current position: Statoil

Torbjørn Gjervan
Studies of bimetallic particle formation in reforming catalysts. Defense of thesis: November 2000
Current position: Research director, SINTEF

Thomas Sperle
Steam reforming of hydrocarbons to synthesis gas.
Defense of thesis: October 2001.
Current position: Chief Technical Officer, Resman

Lucie Bednarova
Study of supported Pt-Sn catalysts for propane dehydrogenation. Defense of thesis: May 2002
Current position: General Motors, Detroit, USA

Sten Viggo Lundbo
Hydrogenation of carbon monoxide over zirconia and modified zirconia catalysts.
Defense of thesis: June 2002.
Current position: Statoil

Leiv Låte
Oxygen-assisted conversion of propane over metal and metal oxide catalysts
Defense of thesis: 2002
Current position: Managing Director, Fedem Technology, Trondheim

Petr Steiner
Kinetic and deactivation studies of hydrodesulfurization catalysts
Defense of thesis: December 2002
Current position: Manager, Hart Energy Consulting, Belgium.

Bozena Silberova
Oxidative dehydrogenation of ethane and propane at short contact time.
Defense of thesis: January 2003
Current position: Docent, Hogeschool Rotterdam, Netherlands

Christian Aaserud
Model studies of secondary hydrogenation in Fischer-Tropsch synthesis studied by cobalt catalysts.
Defense of thesis: May 2003.
Current position: Gassco

Kjetil Hauge
Oligomerization of isobutene over solid acid catalysts for production of high octane gasoline
Defense of thesis: September 2004.
Current position: Statoil

Thomas Løften
Catalytic isomerisation of light alkanes
Defense of thesis: December 2004
Current position: Statoil Mongstad

Zhixin Yu
Synthesis of carbon nanofibers and carbon nanotubes.
Defense of thesis: January 2005
Current position: Statoil

Kjersti O. Christensen
Steam reforming of methane on different nickel catalysts.
Defense of thesis: March 2005
Current position: Statoil research centre. Trondheim.

Ingrid Aartun
Microstructured reactors for hydrogen production.
Defense of thesis: June 2005
Current position: Statoil, Mongstad

Sølvi Storsæter
Fischer-Tropsch synthesis over cobalt supported cobalt catalysts.
Defense of thesis: June 2005
Current position: Statoil, Mongstad

Erlend Bjørgum
Methane conversion over mixed metal oxides
Defense of thesis: January 2006
Current position: Statoil, Mongstad

Vidar Frøseth
A steady-state isoptopic transient kinetic study of Co catalysts on different supports.
Defense of thesis: May 2006
Current position: Statoil, Mongstad

Florian Huber
Nanocrystalline copper-based mixed oxide catalysts for water-gas shift
Defense of thesis: August 2006
Current position: HTE, Germany.

Øyvind Borg
Role of alumina support in cobalt Fischer-Tropsch synthesis.
Defense of thesis: April 2007
Current position: Statoil research centre, Trondheim.

Espen Standal Wangen
Characterisation and pyrolysis of heavy oils
Defense of thesis: May 2007
Current position: Postdoc, NTNU

Hilde Dyrbeck
Selective catalytic oxidation of hydrogen and oxygen-assisted conversion of propane
Defense of thesis: September 2007
Current position: Statoil research centre, Trondheim

Svatopluk Chytil
Platinum supported on mesoporous silica SBA-15: preparation, characterisation and catalytic properties
Defense of thesis: September 2007
Current position: Scientist, SINTEF

Ingvar Kvande
Carbon nanofiber supported platinum catalysts.
Defense of thesis: December 2007
Current position: Researcher, Bioforsk Økologisk, Tingvoll

Hilde Bjørkan
Preparation and characterization of Cu- and Pt-based water-gas shift catalysts.
Defense of thesis: May 2008
Current position: Researcher, SINTEF Trondheim.

Silje Fosse Håkonsen
Oxidative dehydrogenation of ethane at short contact times.
Defense of thesis: June 2008
Current position: Researcher, SINTEF Oslo

Bjørn Christian Enger
Hydrogen production by catalytic partial oxidation of methane.
Defense of thesis: December 2008
Current position: Postdoc, NTNU

Nina Hammer
Au-TiO_2 catalysts supported on carbon nanostructures for CO removal reactions
Defense of thesis: November 2008
Current position: Yara, Porsgrunn

Astrid Lervik Mejdell
Properties and application of 1-5 μm Pd/Ag23wt.% membranes for hydrogen separation
Defense of thesis: May 2009
Current position: Researcher, Statoil

Li He
Sortion enhanced steam reforming of biomass derived compounds
Defence of thesis: January 2010
Current position: Norner, Porsgrunn

Sara Boullosa Eiras
Comparative study of selected catalysts for methane partial oxidation.
Defense of thesis: October 2010
Current position: Postdoc, NTNU

Hamidreza Bakhtiary
Performance assessment of a packed bed microstructured reactor – heat exchanger for methanol synthesis from syngas.
Defense of thesis: November 2010
Current position: Senior researcher, Det norske veritas (DNV).

Xuyen Kim Phan
Catalyst formulations for use in microstructured reactors for conversion of synthesis gas to liquids.
Defense of thesis: January 2011

Fatemeh Hayer
Direct Synthesis of Dimethyl Ether in Microstructured Reactors
Defense of thesis: March 15 2011.

Shreyas Panduran Rane
Relation between Catalyst Properties and Selectivity in Fischer-Tropsch Synthesis
Defense of thesis: May 2011
Current position: Trondheim Forskning og Utvikling (TFoU)

Fan Huang
3D Carbon/polyaniline Nanostructures for Energy Storage
Defense of thesis: August 2011
Current position: Jotun, Sandefjord

Oana Mihai
Partial Oxidation of Methane by Chemical Looping
Defense of thesis: September 2011
Current position: Post.doc. Chalmers, Sweden

Jia Yang
A steady-State Isotopic Transient Kinetic Study of Cabalt Catalysts: Mechanistic Insights and Effect of Cabalt Particle Size, Supports and Promoters.
Defense of thesis: October 2011
Current position: Post.doc. NTNU

Nikolaos E. Tsakoumis
Deactivation of cobalt based Fischer-Tropsch synthesis catalysts
Defense of thesis: November 2011
Current position: Post.doc. NTNU

Kazi Saima Sultana
Calcium Based CO_2 Acceptors for Sorption Enhanced Steam Methane Reforming
Defense of thesis: November 2011

Navaneethan Muthuswany
Platinum based Catalysts for Methanol Fuel Cells: Metal Clusters and Carbon Supports.
Defense of thesis: December 2011