

FASTCARD

Project Meeting 8-9 January 2015 in Chilton, United Kingdom

The EU FP7-funded project FASTCARD had its third meeting with 42 participants from 9 different countries in Chilton on 8-9 January 2015 (Fig. 1). In this meeting, further results were reported, on the first day in different

working group sessions and on the second day in plenary sessions. In the following, a few significant results from the work packages are reported.



Figure 1: Group photo and dinner photo.

Within WP1 (hydrocarbon reforming), four challenges have been identified for the hydrocarbon reforming catalysts: sulfur poisoning, coking, sintering and dust. Various strategies have been developed to meet these challenges.

One option is for example to shield the catalyst by synthesizing transition-metal nanoparticles within hollow zeolite crystals (Fig. 2), which should help to reduce sintering and coking. By using bimetallic catalysts, the sulfur sensitivity should be reduced.



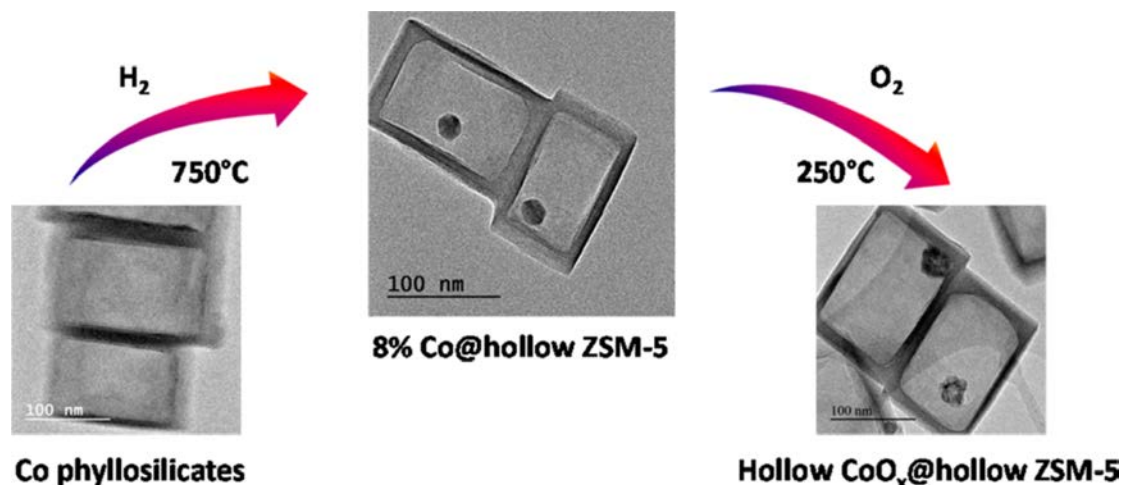


Figure 2: Synthesis of shielded Co nanoparticles within hollow ZSM-5 zeolite crystals (S. Li, A. Tuel, D. Lapruné, F. Meunier, D. Farrusseng, *Chem. Mater.* 27 (2015) 276-282).

Within WP2 (Fischer Tropsch synthesis), both DFT and kinetic models have been developed, which show good agreement with experimental data. New Fe catalysts have been studied. Iron carbide nanoparticles have been synthesized successfully and via a potentially scalable route. These have demonstrated good Fischer Tropsch activity with significantly reduced selectivity to CO₂. Fe catalysts within hollow zeolite frameworks have also been produced. In addition, in situ XANES characterization of the SoA material has given insight into the iron phases present during FT.

Within WP3 (hydrotreating of pyrolysis oils), lifetimes of the catalysts for the stabilization and the partial deoxygenation step of more than 500 h have been reached. The deactivation of the commercial PiculaTM catalyst for the stabilization step has been studied in order to further increase the possible lifetime. For the partial hydrodeoxygenation, new catalysts have been synthesized and analyzed by XPS, TEM and EDX.

Within WP4 (co-FCC of conventional feeds and biooil), a test in the FCC pilot plant with a mixture of 90% vacuum gas oil and 10% fully deoxygenated biooil has been performed. The fully deoxygenated biooil performs actually even better than the conventional fossil feed.

Samples of the thus deactivated state-of-the-art commercial FUTURA catalyst have been distributed to the partners for further analysis and testing. For the development of new catalyst formulations, a small-scale spray drying system has been installed. Experimental facilities for testing the formulated catalyst and the active component are being aligned, also taking into account model feedstocks.

Within the important cross-linking work packages WP5 (nanoscale probing and modelling) and WP6 (conceptual process design and energy efficiency), a lot of alignment work has been done in several joint working sessions together with the other work packages. Within WP5, global kinetic models for hydrotreatment and co-FCC have been refined. The development of single-event microkinetic models has started. Within WP6, different process alternatives were evaluated for the gas value chain. A trickle bed reactor has been selected for hydrotreating.

The meeting ended with a tour through Johnson Matthey's research facilities, where pilot plant and catalyst testing facilities as well as catalyst synthesis and formulation equipment could be visited.

The following pages introduce 4 more partners in greater detail.



SINTEF

Brief description of the organisation and of the department contributing to the execution of the project

SINTEF is one of the largest European research institutes with around 2100 employees and an annual turnover of about 377 mEuro, mainly originating from bilateral industrial research contracts and participation in European or National research projects. The division SINTEF Materials and Chemistry exhibits long term competence within material science, catalysis and process development, and has during recent years been involved in a number of projects related to upgrading of oil and natural gas, including Fischer-Tropsch technology, Methanol-to-olefins, catalytic cracking, single-site catalysis, fuels cells technology, desulphurization, oligomerization and polymerization technologies, dehydrogenation reactions, synthesis and characterization of micro- and mesoporous materials, metal oxides, zeolites, different carrier materials, perovskites etc., separation and purification technologies - among others.

Role in project and previous experience relevant to the task

SINTEF Materials and Chemistry has for many years been involved in different EU projects, including biorefinery related topics within the BIOCAT, AFORE and EuroBioRef projects, dedicated to the development of catalysts for conversion of lignocellulosic biomass to valuable chemicals and fuels. SINTEF's participation to FASTCARD would be related to catalysts development, characterization and evaluation of hierarchical and other porous materials for the conditioning (hydrostabilisation & upgrading) and co-processing of bio oils in FCC with respect to the production of biofuels. We could utilize our materials expertise for developing of novel materials on a small scale.

Person assigned to the project

Duncan Akporiaye (Research Director) with more than 25 years experience in SINTEF on development and characterization of (micro) porous materials. Extensive experience from managing national and international research projects. 10 years experience within the field of High Throughput development and application.

Rune Lødeng (Senior Scientist) has 29 years experience in SINTEF on process technology, catalysis and reaction kinetics (natural gas conversion). Extensive experience on management of national projects.

Ørnulv B. Vistad (Research Scientist) main expertise in synthesis and development of microporous materials and catalysts.

Elisabeth Tangstad (Senior Scientist) has long experience within process technology and catalysis and within managing national and international research projects.

Previous participation in other projects related to this project

SINTEF's Department of "Process Chemistry" has been involved for many years in different EU projects, including biorefinery related topics within the BIOCAT, AFORE and EuroBioRef projects, dedicated to the development of catalysts for conversion of lignocellulosic biomass to valuable chemicals and fuels.

Special Equipment available for the project

We are well equipped with material synthesis and characterization equipment, as well as lab. scale test rigs.



CNRS

Brief description of the organisation and of the department contributing to the execution of the project

The Centre National de la Recherche Scientifique (French National Center for Scientific Research) is a public organization for scientific and technological research and is under the authority of the French Ministry for Research. The CNRS is the largest fundamental research organization in Europe (>25 000 comprising more than 10 000 research scientists). It is also an important breeding ground for scientific and technological innovation.

IRCELYON (Research Institute for Catalysis and Environment of Lyon) is a Joint Research Unit CNRS-Université Claude Bernard and is among the largest French joint laboratory of CNRS and University entirely devoted to catalysis.

The “Engineering and process intensification” (ENG) team (about 30 persons) in charge of this project has already gained a large experience in fossil- and bio-fuel processing including gas and liquid upgrading. ENG is involved both in the combined development of new catalysts and reactors. This integrated approach is carried out by means of mechanistic and modelling studies supported by transient techniques using labelled reactants, in situ DRIFT/Raman/Mossbauer spectroscopies, thermogravimetry/microcalorimetry analysis, all main characterization techniques of solids (XPS, XRD, NMR,..) , and advanced on-line analysis of complex petrochemical liquids and waxes. The laboratory benefits also of cutting-edge equipments available on the campus such as the most powerful NMR (1GHz) and environmental high resolution TEM (300kV) in the world. In addition, the combinatorial and high throughput methodology is routinely applied for the optimisation of existing materials and the establishment of structure-activity relationship by data mining software. Current research topics deal with energy and chemical productions from alternative/sustainable feedstocks by efficient separation and catalytic processes.

Role in project and previous experience relevant to the task

CNRS participation will be related both to catalyst design and testing for the gasification value chain, and to modelling and advanced characterization.

Person assigned to the project

Dr Yves Schuurman is permanent researcher; co-leader of the group ENG, authors of over 70 peer-reviewed papers. He is in charge of activities dealing with natural gas processing (reactor design, kinetic studies and modelling) as well as bio-oils derived feed stocks with petrochemical (naphtas) feed-stocks in refining units.

Dr David Farrusseng is permanent researcher,co-leader of the team ENG, authors of over 100 peer-reviewed papers and 15 patents. He is in charge of activities dealing with i) catalyst design at nanoscale (MOFs, hierarchical structured zeolites and metallic nanoparticle encapsulation) and ii) development of the combinatorial methodology and high throughput parallel reactors.

Dr Frederic Meunier is permanent researcher at CNRS, author of over 70 papers, published in international journals, two patents. He is in charge of the tasks dealing with the in situ characterisation of the catalysts.

Dr Claude Mirodatos is permanent researcher, former leader of the ENG team; author of over 250 peer-reviewed papers in international journals, 15 chapters and reviews. His domain of expertise in line with the FASTCARD project is: natural gas and light alkane activation, syngas cleaning and conversion, biomass and fossil resources FCC co-processing for generating new generation bio-fuels.

Previous participation in other projects related to this project

ANR BIOSYNGOP, BIOCOUP, OCMOL, TOPCOMBI, CARENA.



ECN

Brief description of the organisation and of the department contributing to the execution of the project

ECN is the leading institute for energy research in the Netherlands and in Europe. Its mission is to develop high-level knowledge and technology for a sustainable energy system and to transfer it to the market. ECN Biomass, Energy Efficiency (BEE) research is dedicated to R&D on the thermal conversion of biomass, waste, and coal into power, heat and gaseous & liquid fuels. Furthermore, the department houses experts on process simulation, catalysis, and materials. For ~20 years, ECN has addressed various aspects of the thermal conversion (combustion, gasification and pyrolysis) of biomass, coal and waste in a broad range of national and international projects. A large number of experimental facilities is in use for tests.

Role in project and previous experience relevant to the task

The main role of ECN in FASTCARD is in WP1: generate test results of reforming catalysts in realistic atmosphere. The extensive test park on thermal conversion will be used, together with the on-line and off-line sampling and analysis facilities. ECN has been working on fluidized bed gasification since 1995 with different technologies and thus has deep knowledge on how to influence gas composition, efficiency, fuel flexibility, etc. This will be used in FASTCARD to make sure that the catalytic developments are fitting the overall system as well as technology. The catalytic experts at ECN will be involved in FASTCARD by supplying a catalyst candidate for hydrocarbon reforming (WP1). These experts will also play a crucial role in translating pure catalytic/material results into something fitting technology and gasification processes.

Person assigned to the project

Bram VAN DER DRIFT, since 1995 working on and now technically responsible for gasification and gas cleaning R&D at ECN. Bram is a Chemical Engineer and is mainly involved in gasification technology development. Current EU-participation: Optimash.

Jean Pierre PIETERSE, main expertise is the development of catalysts and sorbents based on metals and metal oxides, zeolites, hydrotalcites and composites, as well as hydrogen production (catalysis) and separation processes.

Previous participation in other projects related to this project

Various projects on fluidized bed gasification and various projects on reforming catalysis for clean hydrogen production.

Special Equipment available for the project

Relevant to this project: 5 kg/h input indirect fluidized bed gasifier ("MILENA") within WP1, a micro-scale catalyst screening and testing facility within WP1 and a 1 kg/h direct fluidized bed gasification and pyrolysis unit ("WOB") to make feedstock for WP4.

References (publications) and patents related to the project

See www.ecn.nl/publications.

1. van der Drift, Biomass gasification for second generation biofuels, Gasification, The development of gasification as a key technology contributor to, London, UK, 19-20 April 2010.
2. R. Smit, Syngas from Biomass, 3rd International Freiberg Conference on IGCC & Xtl Technologies, Dresden, Germany, 18-21 May 2009.
3. J.A.Z. Pieterse, Catalyst for hydrogen production, Patent, WO2012067505.
4. J.A.Z. Pieterse et al. On the potential of Nickel Catalysts for Steam Reforming in Membrane Reactors, Catalysis Today, 2010, 156,3-4, 153-164.
5. D.A.J.M Ligthart, J.A.Z. Pieterse, E.J.M. Hensen, E.J.M.. The role of promoters for Ni catalysts in low temperature (membrane) steam methane reforming. Applied Catalysis. A, General, 2011, 405, 108-119.



Universiteit Gent (UGent)

Brief description of the organisation and of the department contributing to the execution of the project

Ghent University offers high-quality, research-based education in all academic disciplines. The mission of open and democratic education is realized by the availability of social facilities and professional guidance concerning the study career. Pursuing cooperation in research and scientific service, numerous research groups, centres and institutes have been founded over the years. Several of them are renowned worldwide, in various scientific disciplines. Ghent University invests an annual amount of more than 175 million euro in research projects on behalf of public and private partners. The Laboratory for Chemical Technology (LCT) is a unit within the Department of Chemical Engineering (EA12), Faculty of Engineering and Architecture. Chemical reaction engineering and heterogeneous catalysis in general and, in particular, the kinetics of chemical reactions are major research axes in this laboratory, which comprises about 80 people among which 6 full-time equivalents of tenured academic staff and is directed by prof. dr. ir. Guy B. Marin.

Role in project and previous experience relevant to the task

Within FASTCARD, UGent will take a central role in the fundamental modelling activities. The corresponding methodology development is performed as part of WP5 and strongly interacts with the first four work packages focusing in particular on the various model reactions that are being investigated. The activities range from the smallest, ab initio, scale up to the simulation of real-life industrial reactors. Models that are adapted to the needs of the scale at which they are employed will be used and developed. The translation of information between various scales, e.g., via feedstock reconstruction or relumped single-event microkinetics (SEMK) belongs to the core expertise of UGent.

Person assigned to the project

Guy B. Marin: In the lab since : 1997; responsibility: full professor/laboratory director

Experience and background: chemical reaction and reactor engineering

Joris W. Thybaut: In the lab since : 1998; responsibility: full professor

Experience and background: catalytic reaction engineering

Vladimir Galvita: In the lab since : 2010; responsibility: senior scientist

Experience and background: catalysis, chemical reaction engineering

Previous participation in other projects related to this project

OCMOL (coordinator), NEXT-GTL, MULTIMOD, TOPCOMBI, JOULE, THERMIE

Special Equipment available for the project

High throughput kinetics set-up; Temporal Analysis of Products for transient, mechanistic investigations;

catalyst synthesis and characterization equipment; high performance computing infrastructure

References (publications) and patents related to the project

1. Single-event MicroKinetics for coke formation during the catalytic cracking of (cyclo)alkane/1-octene mixtures R. Quintana-Solórzano, J. W. Thybaut, P. Galtier, G. B. Marin *Catalysis Today* 127 (2007) 17-30 SCI-IF: 2.365.
2. Simulation of a slurry-bubble column reactor for Fischer-Tropsch synthesis using single-event microkinetics G. Lozano-Blanco, J.W. Thybaut, K. Surla, P. Galtier, G.B. Marin, *AIChE Journal*, 55 (2009), 2159-2170, SCI-IF: 1.607.
3. Hydrogen Production from Methane and Carbon Dioxide by Catalyst-Assisted Chemical Looping, V. V. Galvita, H. Poelman, G. B. Marin *Topics Catal.* 54 (2011) 907-913 SCI-IF: 2.624
4. Single-Event MicroKinetics: Catalyst Design for complex reaction networks J.W. Thybaut, G.B. Marin, *J. Catal.*, 308 (2013) 352-362 SCI-IF: 5.787

