EUROPEAN COOPERATION
IN SCIENCE AND TECHNOLOGY

Catalysis for the Production of Transportation fuels and chemicals: Innovations and Challenges

Background

The production of liquid transportation fuels such as gasoline, diesel and jet fuel from petroleum involves the use of a variety of catalytic processes. Although the petroleum refining industry is quite mature, fuel composition requirements continue to evolve with time in response to environmental legislation and changes in engine design.
With crude oil reserves decreasing and with increasing concerns about climate change, intense research efforts are being developed all over the world to establish alternatives for the production of transportation fuels and chemicals. Taken together, these changes pose considerable challenges to the refining (and biorefining) industry and significant advances in catalysis are needed to meet the challenge.

1-Towards alternative feedstocks

There are still plenty of natural reserves, such as coal, tar sands and natural gas, for the production of chemicals and transportation fuels. However, the amount of high quality and easily accessible crude oil is decreasing, while heavier feedstocks have to be treated to meet the increasing quality requirements for e.g. transportation fuels. Natural feedstocks, such as methane, methanol and light alkanes, can also be used as the basis for production of fuels and chemicals. Different strategies can be explored. Alternative feedstocks, such as biomass and algae are currently being investigated for the production

of biofuels and (bio-) chemicals to be implemented in future biorefineries.

The production of transportation fuels and chemicals from feedstocks involves the use of a very important chemical process: Catalysis.

2- Enabling Technology : Catalysis

2-1 What is catalysis?

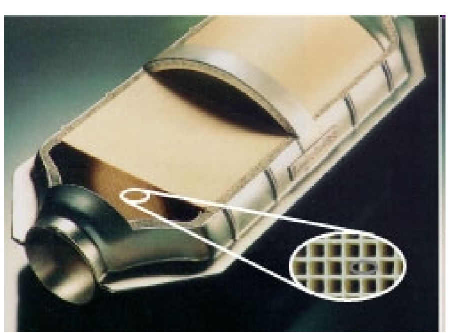
The phenomenon of catalysis is the ability to increase the rate of a chemical reaction, or more specifically the rate at which equilibrium is attained. This is achieved by employing a catalyst, and therefore compared to the none catalyzed reaction, milder operating conditions can be used. The catalyst is not consumed during the chemical reaction, and therefore it is a species that effects change. Catalysts can be divided into two classes; homogeneous catalysts are in the same phase as the reactants, e.g. both are in the liquid phase, while heterogeneous catalysts are in a different phase from the reactants, with most commonly catalysts being solid with gas and liquid reactants. The use of a catalyst also often imparts a degree of selectivity to one or more reaction products, when compared to the non catalyzed reaction. This is an important concept in catalysis, and along with the ability to increase the rate of reaction, both can be manipulated by selection and modification of the catalyst. In conclusion, the use of a catalyst leads to a process that is more energy efficient, uses feedstocks more efficiently, as undesired products are minimised, and pollution is reduced. Hence, catalysis has a crucial role for efficient utilisation of our limited resources in an environmentally responsible manner.

2-2 Economical impact of Catalysis

The value of catalysis, in both impact on quality of life and economic terms, cannot be under estimated. Catalysis underpins many industries; none more so than the chemical industry, as over 90% of chemicals produced rely, to some extent, on the use of a catalyst. The worldwide market for catalysts is large and is growing continually. Current estimates place the value of the catalyst market at >20 billion USD, which is remarkable as it has been estimated that for every 1USD spent on a catalyst it can generate up to 1000 USD worth of product. Four of the world's most successful industrial sectors are petroleum, chemicals production, energy generation and food production, and all of these industries rely heavily on catalysis, with their worldwide GNP accounting for at least 10 trillion USD. The importance of catalysis is mirrored across many sectors and estimates suggest that catalysis contributes to >35% of the world's GDP. Against this background, it is clear that catalysis is an important key enabling technology that supports our economies. It would be difficult to imagine life without modern synthetic polymers, as they are used for diverse applications including paints, adhesives, packing, textiles/fibers, electronic and biomedical devices. All of these materials depend on catalysis for their production.

2-3 Importance of catalysts in fuel production and challenges for alternative feedstocks

The applications of catalysis are numerous, and impact heavily on our daily lives. The process of fluidized catalytic cracking (FCC) is the heart of the modern oil refinery and uses a catalyst to convert crude oil to lower boiling fractions that can be used as gasoline, diesel, aviation fuel and fuel oil, as well as a wide range of chemical feedstocks, which can be transformed further using a host of other catalytic processes to produce many essential chemicals for a wide variety of applications. Catalysts are also used for protection of the environment, and many will be familiar with the



catalytic converter, which is now fitted as standard to many vehicles around the world, reducing emissions of deleterious carbon monoxide, hydrocarbons and nitrogen oxides.

Catalysis will play a pivotal role for the generation of clean fuels, like hydrogen, and energy production using highly efficient fuel cells. Catalytic technology will also be central for implementation of more efficient and greener manufacturing processes. It will also be crucial for initiating new sustainable manufacturing processes by utilizing alternative feedstocks, such as non-edible biomass. Catalysis is a multidisciplinary field and contains engineers and scientists from chemistry, materials science, physics, biology and biochemistry. It provides the opportunity to work on fundamental problems, the 2007 Nobel Prize for Chemistry was awarded to G. Ertl for his work on heterogeneous catalysis, as well as important applied aspects.

Scientific rationale

Heavy and dirty feedstocks require catalysts for removal/decomposition of poisonous molecules and for removal of heavy metals. Can these processes be combined in one catalyst? This “ideal” catalyst fixes the heavy metals in such a way that they serve as catalytic sites for decomposition/removal of the poisonous molecules. In addition, the catalyst contains the acid sites necessary for cracking/isomerization of the long chain hydrocarbons.

In catalysis it is important to avoid poisoning (oxidation) of the catalyst by polar molecules (oxygen). The “ideal” catalyst takes oxygen atoms “out of the polar molecules” and stores them in its structure in such a way that the catalyst can activate the reaction; i.e., the conversion of biomass into fuels and basic chemicals.

For methane and light alkanes conversion catalytic research boils down to “selectivity”: selective activation of a carbon-hydrogen bond with avoidance of complete burning of methane and other light alkanes into carbon dioxide and water.

The ideal catalysts possessing the required activity, selectivity and stability do not yet exist, except maybe for the enzymes that selectively activate methane by insertion of an oxygen atom in the carbon hydrogen bond (C-H). We must rely on:

(1) The construction of improved catalyst materials, which are designed by either combinatorial methods or rational catalyst design, based on e.g. theory and advanced characterization methods;

(2) The intelligent combination of different types of catalysts or different types of active sites in one catalyst, making use of the respective strengths of these active sites and the catalysts materials. All combinations should be allowed: enzyme + heterogeneous catalyst; homogeneous + heterogeneous catalyst; Furthermore, photocatalysis also comes into the picture;

(3) Alternative reaction media in which catalytic and separation technologies are combined. Examples include catalysis in ionic liquids, in supercritical conditions, etc. In this way, unreactive aggregates of molecules can be disentangled into monomolecular or oligomeric entities, which are more susceptible to catalytic attack.

Finally, whatever the catalytic process being developed, the question will be raised on its sustainability, its impact on the environment and on the climate. The economical, environmental and social impact of such process must be evaluated before production can start. Scientists must take these considerations into account in multidisciplinary studies.

2-4 European Technology Platforms

In February 2009, the European Parliament resolution "2050: The future begins today – Recommendations for the EU's future integrated policy on climate change" (2008/2105(INI)) set out a range of measures that should be taken in order to reduce greenhouse gas emissions by 25-40% by 2020 and a reduction of at least 80% by 2050.

Among other measures, the resolution advocates that EU Member States should invest in research on sustainable advanced biofuels.

The European Strategic Energy Technology Plan (SET-Plan) (January 2007) aims to match the most appropriate set of policy instruments to the needs of different technologies at different stages of the development and deployment cycle. It addresses the entire innovation process from basic research to market uptake for bioenergy, including biofuels.
In October 2009, the EC published a proposal on Investing in the Development of Low Carbon Technologies (SET Plan), calling for an additional €50bn investment in low carbon technologies, including €9bn for bioenenergy (advanced biofuels and efficient CHP).
2 out of many European Technology Platforms, which have been created in order to answer the future challenges the energy/fuel industry will face in the coming years, are directly concerned by the topics of the workshop.

The **European Biofuels Technology Platform (EBTP)** will contribute to the development of cost-competitive world-class biofuels value chains and the creation of a healthy biofuels industry, and to accelerate the sustainable deployment of biofuels in the European Union, through a process of guidance, prioritisation and promotion of research, technology development and demonstration.
http://www.biofuelstp.eu/index.html

The **Zero Emission Platform (ZEP)** created in 2005 has for objectives to:

1. **Enable CCS (CO_2 Capture Storage) as a key technology for combating climate change.**

2. **Make CCS commercially viable by 2020 via an EU-backed demonstration programme.**

3. **Accelerate R&D into next-generation CCS technology and its wide deployment post-2020.**

Over 200 people from 19 countries actively contribute to ZEP's activities in its role as:

- **CCS Advisor and Facilitator** – expert advice on all technical, policy, commercial and other related issues.

- **CCS Technology Contributor** – input on all technology issues, including recommendations for next-generation technologies, taking into account experience gained from the EU CCS Demonstration Programme.

- **Respected communicator** – educator and authoritative source of information, while being engaging internationally on CCS.

http://www.zeroemissionsplatform.eu/extranet.html

Those 2 platforms will be participating actively to the discussion.

2-5 COST involvement in Catalysis

COST Actions are strongly involved in catalytic research and will benefit greatly of this workshop and especially the starting Action CM0904 which could have the kick off meeting following this Workshop.

D36 Molecular structure-performance relationships at the surface of functional materials

The main objective of the Action is to increase the fundamental knowledge and understanding of the chemistry occurring at surfaces and interfaces and the factors that tune it. An interdisciplinary, combined effort is the approach. A fundamental approach is advocated, even for industrially oriented research projects. 22 countries are represented in this Action.

CM0903 Utilisation of Biomass for Sustainable Fuels & Chemicals

The main objective of the Action is to generate a synergistic approach for utilisation of biomass for sustainable fuels & chemicals through cooperation between scientists from different member states and different areas and disciplines. 19 Countries are already represented in this Action which started in November 2009.

CM0904 Network for intermetallic compounds as catalysts for steam reforming of methanol.

The main objective of this Action is to establish a dedicated platform and a knowledge-based approach for the development of intermetallic compounds as methanol steam reforming catalysts. The deep understanding of the underlying processes will enable a rational development of catalysts with high economic impact. The Committee of Senior Officials (CSO) approved the Action on December 2, 2009.

Action CM0901: Detailed chemical kinetic models for cleaner combustion

The main objective of the Action is to develop cleaner and more efficient combustion processes through the design and implementation of better defined and more accurate detailed chemical kinetic models. The key objective of this Action is to promote at EU level the development of cleaner and more efficient combustion technologies through the implementation of theoretically grounded and more accurate chemical models. This Action will have its first kick off meeting on January 28-29 2010.

3- Conclusion

In the proposed workshop, scientists will discuss the catalysis and catalytic processes to convert the broad variety of alternative feedstocks (biomass, methane, ethane, very heavy crude and coal, methanol, carbohydrates, algae, glycerol) into transportation fuels and chemicals. After introducing the state of the art in the catalytic field and in different domains, the performance of new catalysts in development and at laboratory-scale will be presented and discussed. The effect of impurities and poisons, present in the alternative feedstocks, on the performances of existing catalysts materials will be explored and new challenges for improving these materials will be presented. In addition, several routes will be designed to approach the "ideal" multifunctional catalyst or the "most appropriate" combination of "ideal" catalyst materials to convert these feedstocks. The role of tools of investigation, of in situ spectroscopic observation of catalysts in action and of theory in this process of catalyst development will be highlighted. Finally, the socio-economic implications in using these alternative feedstocks will be presented.

ORGANIZATION

Organization Committee

Prof. em. Robert Schoonheydt, K.U.Leuven, Belgium: chair

Prof. Rutger van Santen, Technical University Eindhoven, The Netherlands

Prof. Bert Weckhuysen, University of Utrecht, The Netherlands

Prof. Miguel Banares, CSIC, Spain, president management committee of COST D36

Workshop organization

We envisage a two-day, Gordon-style workshop with key-note speakers only, covering the various aspects of the subject. COST Chemistry is the European umbrella organization under which this workshop is operated. However, as the scientific problems associated with sustainable production of transportation fuels and chemicals are global, the organizing committee seeks active participation of scientists and scientific organizations from Asia and America. Individual participants can contribute to the workshop with a poster.

The workshop is organized into four themes. Each theme is covered by three to five key-note speakers. Each speaker has one hour with 45 min to present his/her relevant data and insights and 15 min of discussion. Some contributions will be 45 min or 30 min. A book of abstracts and a list of participants will be distributed to facilitate contacts and discussions.

Theme 1: Heavy Feedstock: Coal and Tar Sands

There are huge reserves of coal and tar sands in the world. Their use as transportation fuel as well as bulk chemicals requires sustainable and economically viable production routes. The production of syngas, followed by Fischer-Tropsch synthesis, is an option currently explored at large scale. Sustainable production also means that added value has to be given to impurities and waste, which come in large quantities with the processes of coal and tar sand upgrading.

INVITED SPEAKERS

Prof. Yongwang Li, Chinese Coal Institute

Prof. Murray Gray, University of Alberta, Scientific Director for The Centre for Oil Sands Innovation

Prof. Erik van Steen, University of Cape Town, South Africa,

Theme 2: *light alkanes*

Methane is an excellent energy source. Its use as a basic feedstock for the chemical industry is challenging due to the strength of the C-H bond and the need for highly selective reactions in order to avoid complete burning to water and carbon dioxide. Inspiration comes from enzymatic catalysis with Cu-containing enzymes.

Invited speakers:

Prof. Edward Solomon, Stanford University

Prof. Unni Olsbye, University of Oslo

Dr. R. Rostrup-Nielsen, Haldor Tøpsoe,

Prof. J. Lercher, Technical University Munich

Theme 3: *Biomass and renewables*

Biomass and renewable feedstocks are proposed as alternatives for fossil fuels. Aspects to be discussed are catalysis, chemical technology and biotechnology.

Invited speakers

Dr. Conrad Zhang, KiOR

Prof. John Regalbuto, NSF and University of Illinois at Chicago

Prof. Bert Sels, K.U.Leuven

Prof. Jim Dumesic, University of Wisconsin

Theme 4: Assessment

New processes and new technologies have to be evaluated for their financial, economical and societal impacts. Are these processes and technologies sustainable? How is this measured, quantified?

Invited speakers:

Prof. Roger Sheldon, TUDelft

Prof. A. Faaij, University of Utrecht

A representative of the EU commission

Timing: Monday-Wednesday April 26-28, 2010

Monday, April 26, 2010

1.30pm: welcome and opening: Robert Schoonheydt, K.U.Leuven

1.45-2.30pm: G. CENTI, president of IDECAT

Renewable Catalytic Processes

SESSION ON HEAVY FEEDSTOCK

2.30 – 3.30 pm: Y. LI, Chinese Coal Institute

From Coal to Liquids

3.30 – 4.00 pm: coffee

4.00 – 5.00 pm: M. GRAY, University of Alberta and Center for Oil Sands Innovation

Tar Sands as Feedstock for Fuels and Chemicals

5.00 – 6.00 pm: E. Van Steen, University of Cape Town

Fischer-Tropsch Chemistry

6.00 – 8.00 pm: **POSTER SESSION**

Tuesday, April 27, 2010

SESSION ON GASES

8.30 – 9.30 am: E. SOLOMON, Stanford University

Cu-enzymes and Cu-zeolites for the selective transformation of methane to methanol

9.30 – 10.30 am: J. LERCHER, Technische Universität München

Elementary steps of C-H activation

10.30 – 11.00 am: coffee

11.00 – 12.00 am: U. OLSBYE, University of Oslo

Mechanisms of the MTO process

12.00 – 1.00pm: R. ROSTRUP-NIELSEN, Haldor Tøpsoe

Reforming of methane: from chemistry to technology

1.00-2.30 pm: lunch

Session on Renewables

2.30-3.00 pm: J. REGALBUTO, University of Illinois at Chicago

An NSF perspective on hydrocarbon biorefineries

3.00-4.00pm: J. DUMESIC, University of Wisconsin

Catalytic Strategies for the Conversion of Biomass-derived Carbohydrates to Liquid Hydrocarbon Fuels

4.00-4.30pm: coffee

4.30-5.30 pm: B. SELS, K.U.Leuven

From Glycerol to Chemicals

5.30 – 6.00 pm: C. ZHANG, KiOR

Conversion of cellulose to oxygenates over Cr catalysts

7.00 pm: **Dinner**

Wednesday, April 29, 2010

SESSION ON ASSESSMENT

9.00-9.30am: R. SHELDON, Technical University of Delft

Metrics of Green and Sustainable Conversion of Biomass to Fuels and Chemicals

9.30-10.30 am: A. FAAIJ, University of Utrecht

10.30 – 11.00am: coffee

11.00-11.30am: EU Commissioner

11.30-11.45 am: **Closure**

11.45-12.30am: **reception**

12.30 pm: lunch

Site of the workshop

THERMAE PALACE HOTEL, Koningin Astridlaan, 7, 8400 Oostende

http://www.thermaepalace.be

sales@thermaepalace.be

POSTERS

Individual scientists and research groups can participate in the workshop with a poster contribution. Posters will be on display during the full time span of the conference. The authors are expected to be present at their poster on Monday, April 26 from 6pm to 8pm for discussions and answering questions. Title of the poster, the authors' names and affiliation and an abstract (max. one page) must be submitted by email before February 28, 2010. The email address is: steven.corthals@biw.kuleuven.be.

ASSESSMENT SESSION

The session on assessment on Wednesday, April 29, 2010 will be open to a larger audience, including policy makers, scientific journalists. Policy makers and journalists will be invited by the organizational committee

SECRETARIAT

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