

FISCH Thematic Workgroup "Catalysis"

Date : 10/03/2009
From : B.Sels/B. Moens
To : Core team FISCH
CC : K. Van Aken
Subject: Thematic workgroup on "Catalysis" dd. 19/02/09
Attach. :

On February, 19th, 2009, a Thematic Workgroup (TWG) Meeting was organized by essenscia in the framework of the FISCH IWT Feasibility Study at GUGA, Diegem (Brussels). Four different TWGs on 1) Catalysis, 2) Novel process technologies, 3) Petroleum replacement, and 4) Product design/intensification individually discussed possible breakthrough projects for their technical theme and built roadmaps for these breakthrough projects. In this Technical Report, the findings of the TWG on "Catalysis" are summarized.

*The major outcome of the Thematic Workgroup Meeting was that a visionary project for "Catalysis" could be: **Selective, catalytic activation of C-X***

- o Bulk chemistry: Development of sustainable CO₂/CH₄ chemistry with minimal energy input (C₁ chemistry)
- o Fine chemistry: activation of various C-X (artificial photosynthesis?)

The contribution of this project to a sustainable chemistry can be:

- *Introduction of new workhorses (microorganisms, algae, fuel cells...)*
- *Development of new, chemical transformations and structures*
- *Development of new, sustainable processes*

1. Attendees

Industry

BASF:	Emile De Decker
BP Chembel:	Stefan Leurs
Cytec:	Luc Boogaerts
Ecosynth:	Koen Van Aken
ExxonMobil:	Marcel Janssen
Ineos:	Joos Wahlen
Proviron:	Marc L'Abbé
Taminco:	Peter Roose
Total:	Pol Hoorelbeke

Knowledge-based Centers

Hogeschool West-Vlaand.:	Tim Vermeiren
KULeuven:	Bert Sels (FISCH Core team member)
KULeuven:	Bart Moens (FISCH Core team member)
Universiteit Antwerpen:	Bert Maes
Universiteit Antwerpen:	Vera Meynen
Universiteit Gent:	Tom Desmet
Universiteit Hasselt:	Koen Smets
VUB:	Kourosch Abbaspour Tehrani
VUB:	Eileen Dejaegere
VUB:	Wim Versees
VUB:	Joeri Denayer
VUB:	Luc De Vuyst

Facilitator

BECO:

2. Introduction

On the basis of initial response, gained by a written questionnaire among all FISCH participants, a compilation of relevant research themes and breakthrough domains in the field of sustainable chemistry was made by Carl Van der Auwera (essenscia). The outcome of this compilation was presented at the Start Event of FISCH on December, 17th, 2008. On the basis of this compilation, four different major **breakthrough domains** could be identified, more specific:

1. Catalysis
2. Novel process technologies
3. Petroleum replacement (using biomass feedstock)
4. Product design/intensification.

For each of these major breakthrough domains, a Thematic Workgroup (TWG) was organized to further elaborate on these themes. For the breakthrough domain/TWG on "**Catalysis**", the following **relevant research themes** were identified on the basis of the questionnaire:

- Homogeneous catalysis (including recuperation and recycling)
- Non-conventional activation and energy sources (microwaves, light, ultrasonic waves)
- Enzymatic reactions
- Nanocatalysis
- Artificial photosynthesis (*i.e.*, with TiO₂)
- CO₂ activation
- Activation of C-H (homogeneous catalysis), *i.e.*, direct conversion of CH₄ to CH₃OH
- Selective (de)functionalization and (de)polymerization of biomass/waste (marriage chemo- and biocatalysis)

In addition, on the basis of these relevant research themes, some possible **breakthrough projects** were identified and compiled by Carl Van der Auwera (essenscia) before the TWG came together. For the TWG on "Catalysis", the following possible breakthrough projects were already identified:

- Reduction of CO₂ and NO_x at 15°C
- Activation of C-H at 15°C
- Flemish catalysts (produced from Flemish resources)
- (De)functionalization and (de)polymerization of biomass

3. Identification of one visionary breakthrough project

The aim of the first part of the TWG session was to define one major (visionary) breakthrough project in the field of "Catalysis".

The meeting was started by Bert Sels (KULeuven), who gave a short, general introduction on catalysis, covering both opportunities, needs and bottle-necks for catalysis in the future.

After the presentations, the attendees discussed about the possibilities of integrated or visionary projects for Flanders within the breakthrough domain "Catalysis". The difference in interests and targets between the bulk chemistry and fine chemistry became quickly obvious. Presentation of one visionary project for the breakthrough domain "Catalysis" is therefore quite complicated.

The most important aspects mentioned by the attendees in the discussion on possible projects for Flanders were as follows:

- Bulk *versus* fine chemistry: improving existing processes and use of CO₂/CH₄ as alternative resources in the latter or innovative research into new processes (*i.e.*, enzyme engineering, catalyst synthesis...)? High-throughput synthesis *vs* intelligent synthesis!
- Petrochemistry in the future: will Flanders still be competitive within 15-20 years or do we need to invest in new, visionary projects (*i.e.*, alternative feedstocks, photosynthesis...)?
- Capital investment: can currently used infrastructure still be used in the future?
- Improving the energy efficiency of currently used processes: sustainable chemistry also means "with minimal energy input"!
- Modelling and upscaling is critical for every catalytic process!
- Ambition of FISCH should be "from development to realisation": Flemish initiatives should be anchored in Flanders!
- Scientific challenge *versus* economic realization
- Further development of Flanders strong points, material synthesis (fundamental) and membrane research (applied), is critical!
- New possibilities: use of micro organisms, algae, fuel cells, new type of catalysts...
- Catalysis is a tool! The exact identity (bio-, homogeneous, heterogeneous, fermentation...) is not important.

The conclusion of the general discussion/brainstorming for the breakthrough project in the field of "Catalysis":

- Splitting bulk- (C₁ chemistry) and fine chemistry (broader scope)
- Target: development of innovative processes
 - Innovative = sustainable, selective, high reaction rate, type of catalysts...
- A possible visionary project could be: **Selective, catalytic activation of C-X**
 - Bulk chemistry: Development of sustainable CO₂/CH₄ chemistry with minimal energy input (C₁ chemistry)
 - Fine chemistry: activation of various C-X (artificial photosynthesis?)

4. SWOT-analysis and Roadmap

In the afternoon session of the TWG Meeting, a SWOT analysis and a preliminary Roadmap for the visionary project were developed by the attendees. This preliminary Roadmap is the starting point for future activities, including regular updates to the Roadmap itself, and the programming of activities to prepare and enable biobased feedstock in the Flemish chemical industry.

The results of the SWOT analysis are presented below.

SWOT- Catalysis	
STRENGTH	WEAKNESS
<ul style="list-style-type: none"> • High concentration and quality of knowledge institutes and industries • Geographical location of Flanders • Excellent technical support • Broad catalytic expertise (both chemo- and biocatalysis) • Broad catalytic technology (membranes, fuel cells...) and knowledge • Sorting out of waste: possible source of chemicals by gasification • Organic synthesis (chiral synthesis, stereoselectivity...) for the fine chemistry • (Fundamental) knowledge of enzymatic catalysis 	<ul style="list-style-type: none"> • Communication • Concurrency • Feasibility of CO₂ conversion • Return-on-investment • Fragmentation of research + lack of strategy and vision • Availability of energy sources • Industrial research mostly in foreign countries • Insufficient sustainable policy around sustainability • Lack of entrepreneurship • Availability of sunlight
OPPORTUNITIES	THREATS
<ul style="list-style-type: none"> • Flanders versus European dimension • Exploitation of new resources • Sustainability • Implementation biomass/resources • Industrial cooperation and knowledge exchange • Research platform • Grow potential in Flanders • Reorientation of research groups and cooperations • CO₂ network in Flanders • Stimulation of homogeneous catalysis for fine chemistry • Application of enzymatic catalysis • Implementation of new technologies in pharma sector • Research focus: alternatives for available chemical infrastructure 	<ul style="list-style-type: none"> • Political instability • Ecology versus economy • Knowledge of resources • Demands of chemistry versus food industry for biomass • Expensive catalytic development for fine chemistry • Availability of sunlight • Brain drain

End of Report