Multi-scale Modeling and design of chemical Reactions and Reactors

M2dcR2

Guy B. Marin

http://www.lct.ugent.be
8h15 | Welcome/ Coffee
8h30 | Excused/Introduction
8h40 | Minutes meeting 17/06/2011 (sent on 07/07/2011)
8h50 | Status of the M2dcR2 programme at midterm (GBM)
9h50 | P1-P3 Single-Event MicroKinetics (SEMK) in complex reaction mixtures, Catalyst design based on catalyst descriptors & Adsorption by nanoporous materials (JT)
10h35 | **coffee break**
11h00 | P5 Reactor design from first principles (GH)
11h45 | Introduction to posters (1 minute each)
12h00 | Lunch/Posters
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
</tr>
</thead>
<tbody>
<tr>
<td>13h45</td>
<td>P1 “Biomass to Olefins: Steam Cracking of Renewable Feedstocks” by Steven Pyl</td>
</tr>
<tr>
<td>14h05</td>
<td>P2-P3 “the catalytic performance of Vanadium based Metal Organic Frameworks in the oxidation of cyclohexene” by Karen Leus</td>
</tr>
<tr>
<td>14h25</td>
<td>coffee break</td>
</tr>
<tr>
<td>14h40</td>
<td>P5 “Multi-scale modeling and reaction path analysis of benzene hydrogenation on Pd(111)” by Gonzalo Canduela</td>
</tr>
<tr>
<td>15h00</td>
<td>P6 “Application of microreactor technology for the modification of renewable resources” by Ana Cukalovic</td>
</tr>
<tr>
<td>15h20</td>
<td>next meeting: date /format</td>
</tr>
<tr>
<td>15h30</td>
<td>feedback/ concluding remarks</td>
</tr>
<tr>
<td>16h15</td>
<td>end of meeting</td>
</tr>
</tbody>
</table>
Advisory Board

- Christopher Barner-Kowollik (KIT; G)
- Rodney Fox (Iowa State; USA)
- William H. Green (MIT; USA)
- Egbert Lox (Umicore; B)
- Philippe Sautet (ENS-Lyon, F)
- Jaap Schouten (TUEindhoven; NL)
- Bert Weckhuysen (U Utrecht, NL)
Organizational aspects

• **Scientific director**: leader of the research group
  • responsible for expenditures, research policy and daily management of the research group

• **Management committee**
  • president: leader of the research group
  • members: at least faculty of the research group
  • manages the research
  • defines the research policy
  • installs an advisory board

• **Advisory board (internationally recognised authorities)**
  • supports in mapping out long term research policy
  • supports in defining research priorities
M2dcR2: management committee (MC)

Three faculties of Ghent University are represented in management committee

• **Engineering:** Laboratory for Chemical Technology (LCT)
  - Prof. G. Heynderickx: reactor hydrodynamics
  - Prof. M.-F. Reyniers: ab initio radical and catalytic chemistry
  - Prof. J. Thybaut: catalytic reaction kinetics and reactors
  - Prof. K. Van Geem: thermal reaction kinetics and reactors

• **Bioscience engineering:** Synthesis and Bioresources Chemistry (SynBioC)
  - Prof. C. Stevens: microreactors and renewable feedstocks

• **Sciences:** Centre for Ordered Materials, Organometalics and Catalysis (COMOC)
  - Prof. P. Van der Voort: catalyst synthesis and design
Objective

“to provide stable and substantial funding to the leader of a research group with a proven track record of excellence that can independently and flexibly be used to acquire and/or strengthen a leading position of the group at an international level”
Methusalem programme: evaluation criteria

- Quality of work
  - performed work outstanding at an international level?

- Human resources management
  - post-doctoral researchers are stimulated to set-up independent research?

- Research plan for next 7 years
  - research plan and funding applied for is adequate?
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Multi-scale Modeling and design of chemical Reactions and Reactors

Guy B. Marin

http://www.lct.ugent.be
Aim M2dcR2: world top centre at UGent

“establishment of unique platform for fully integrated and knowledge based design of products and processes”

Methusalem proposal presentation, 11 September 2008
M2dcR2: **multi-scale** modeling and design
from atom (nm) to full process (m)
M2dcR2: strategy

• **Design** of sustainable products and processes guided by:

  modeling of complex kinetics

  combined with

  complex transport phenomena

  based on:

  • first principles
  • experimental validation

• **Renewable feeds**

  • transportation fuels and energy carriers
  • chemicals
  • functional materials (catalysts, nanostructured polymers)
Modeling and design of reactions and reactors

process

product

transport

mixing
diffusion
momentum transport
structured microreactors
rotary bed

reactor modeling and design

reaction modeling and design

chemistry

reaction network generation
kinetics
reaction rules
catalysis
adsorption
catalyst descriptors
controlled polymerization
M2dcR2: application domains

- biomass to liquids
- renewables to chemicals
- environmental
- functional materials
  - catalysts
  - polymers
LCT: people

- Part-time professors: 2
- Visiting/senior scientists: 4
- Post-docs: 8
- PhD students: 28
- Technical staff: 8
- Administrative staff: 2
<table>
<thead>
<tr>
<th>Subprogramme</th>
<th>MC member</th>
</tr>
</thead>
</table>
| **P1** | J. Thybaut  
|  | M.-F. Reyniers  
|  | K. Van Geem |
| **P2** | J. Thybaut  
|  | M.-F. Reyniers  
|  | P. Van der Voort |
| **P3** | J. Thybaut  
|  | M.-F. Reyniers |
| **P4** | G. Heynderickx, M.-F. Reyniers, P. Van der Voort |
| **P5** | G. Heynderickx  
|  | C. Stevens |
| **P6** | C. Stevens, J. Thybaut, M.-F. Reyniers, K. Van Geem |
M2dcR2: subprogrammes

- Single-Event Microkinetics (SEMK) in complex reaction mixtures (P1)
- Catalyst design based on catalyst descriptors (P2)
- Adsorption by nanoporous materials (P3)
- Polymer design accounting for mixing and diffusion (P4)
- Reactor design from first principles (P5)
- From fossil to renewable feedstocks (P6)
<table>
<thead>
<tr>
<th>PhD</th>
<th>research topic</th>
<th>advisors</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steven Pyl</td>
<td>Light olefins from fossil and renewable resources by thermal routes (P1; P6)</td>
<td>GBM; MFR</td>
</tr>
<tr>
<td>K. Alexopoulos</td>
<td>Total oxidation of propane by anorganic oxides (P2-P3)</td>
<td>GBM; MFR</td>
</tr>
<tr>
<td>Karen Leus</td>
<td>V containing MOF’s for selective oxidations (P2-P3)</td>
<td>PVDV; GBM</td>
</tr>
<tr>
<td>Carolina Toloza</td>
<td>Kinetic modeling of controlled radical polymerization (CRP) (P4)</td>
<td>GBM; MFR</td>
</tr>
<tr>
<td>Ana Cukalovic</td>
<td>Use of structured microreactors for, in decreasing order of priority: coupling of amino acids, addition of cyanide to ketones or aldehydes, amino substituted isosorbide derivatives (ionic liquids), derivatization of hydroxymethylfurfural (P5)</td>
<td>CS; GH</td>
</tr>
<tr>
<td>Jelena Kovacevic</td>
<td>Process intensification by high-g reactor technology for gas-solid reactions (P5)</td>
<td>GBM; GH</td>
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## funded PhD’s

<table>
<thead>
<tr>
<th>PhD</th>
<th>research topic</th>
<th>advisors</th>
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<tbody>
<tr>
<td>Marco Djokic</td>
<td>Model steam cracking of gas oils, waxes and vacuum gas oils (P1)</td>
<td>GBM;KVGG</td>
</tr>
<tr>
<td>Jeroen Lauwaert</td>
<td>Model based design of bifunctional acid/base catalysts for aldol condensations (P2-P3,P6)</td>
<td>(JT,PVDV,GBM)</td>
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<tr>
<td>Gaoping Xue</td>
<td>Assessment of new FCC technology (MIP) using single-event microkinetics (P1)</td>
<td>GBM;JT</td>
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<tr>
<td>Gonzalo Canduela</td>
<td>Multi-scale modeling of benzene hydrogenation on Pd-based bimetallic catalyst (P2-P3)</td>
<td>GBM;MFR</td>
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<tr>
<td>Mike Nguyen</td>
<td>Ab initio Study of the Zeolite-Catalyzed Conversion of Oxygenates (P2-P3, P6)</td>
<td>GBM;MFR</td>
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# Funded Postdoctoral Scientists

<table>
<thead>
<tr>
<th>Postdoctoral Scientists</th>
<th>Research Topic</th>
<th>Subprogram</th>
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</thead>
<tbody>
<tr>
<td>Robert Ashcraft</td>
<td>Computational research on rotating powder flow</td>
<td>P5</td>
</tr>
<tr>
<td>Maria Pantzali</td>
<td>Computational and Experimental research on powder flow</td>
<td>P5</td>
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<tr>
<td>Tatyana Glazneva</td>
<td>Study of the methane dry reforming mechanism by spectroscopic and transient kinetic experiments</td>
<td>P2-P3</td>
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<tr>
<td>Hans-Heinrich Carstensen</td>
<td>Ab initio calculation of rate coefficients of gas phase reactions</td>
<td>P1</td>
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## Senior Scientists

<table>
<thead>
<tr>
<th>Senior Scientists</th>
<th>Research Topic</th>
<th>Subprogram</th>
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<tbody>
<tr>
<td>Hilde Poelman</td>
<td>Physical Characterization Techniques, in particular XAS</td>
<td>P2-P3, P6</td>
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<tr>
<td>Denis Constales</td>
<td>Mathematical methods for reaction and reactor engineering</td>
<td>P1-P5</td>
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<tr>
<td>Equipment</td>
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<td>MadpII</td>
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<td><strong>Total</strong></td>
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</table>
P1: Microkinetics (SEMK)

- Gas phase reactions
  - Ab initio simulation of ethane steam cracker
  - Heteroatoms: O, S, Si
  - Stereochemistry
- Catalytic reactions
  - Ab initio calculations on zeolites
  - Reaction network generation on metals
  - Coke deposition
  - Oxidation of hydrocarbons
- Feedstock reconstruction
  - Principal Component Analysis
  - Shannon Entropy Maximization
  - Constrained Homologous Series
P2: Model based catalyst design

1. new concept
2. performance testing
3. industrial application
4. design

- catalyst library
- activity library
- optimized descriptors
- kinetic and catalyst descriptors
- synthesis
- modelling
P2: Catalyst design

- Acid catalysis
  - “extreme” shape selectivity in zeolites
  - patent assigned to Nippon Oil
- Catalyst descriptors
  - Fischer-Tropsch
  - Oxidative Coupling of Methane
- Catalyst synthesis
  - Zeolites, Metallo-Organic Frameworks (MOF’s)
  - Periodic Mesoporous Organosilica (PMO’s)
  - Anorganic oxides: identification of active sites
Control of pore diameter and functionality

Periodic Mesoporous Organosilicates (PMO)
Ways to make acid catalysts

SULPHONATION

Aromatic sulphonation

Aliphatic sulphonation

i. SULPHONATED MESOPOROUS PHENOLIC RESIN

ii. 

iii. 

iv. 

For aromatic groups

For hydroxyl groups
Sequence of reactions for toluene total oxidation:

- Toluene adsorbs parallel to the surface of the catalyst
- Simultaneous abstraction of H atoms to form $\text{H}_2\text{O}$
- Abstraction of C from the methyl group to form $\text{CO}_2$
- Destruction of the aromatic ring to form $\text{CO}_2$

Toluene total oxidation is very sensitive to the degree of reduction of the catalyst.

Importance of weakly bound oxygen forms present in fully oxidized catalyst
TEM of CuCeAl

2 morphologies:

- Ceria nanocrystals (~6 nm) agglomerated into ~100 nm
  - Ring pattern in SAED
  - Fit with CeO$_2$ lattice

- CuO monocrystals ~100nm
  - Spot pattern in SAED

EDX
15% of total Cu present in CeO$_2$ agglomerates
Cu:Ce ≈ 1:2
CuO-CeO$_2$/Al$_2$O$_3$

Cu$_x$Ce$_{1-x}$O$_{2-x}$ solid solution: activity, reducibility?
Solid solution

\[
\text{Tol} + \text{Cu}^{2+} \rightarrow \text{Cu}^0 + \text{CO}_2 + \text{H}_2\text{O}
\]
\[
2\text{Ce}^{4+} + \text{Cu}^0 \rightarrow 2\text{Ce}^{3+} + \text{Cu}^{2+}
\]
\[
2\text{Ce}^{3+} + \text{O}_2 \rightarrow 2\text{Ce}^{4+}
\]

and/or

\[
\text{Ce}^{3+} + \text{H}_2\text{O}/\text{CO}_2 \rightarrow \text{Ce}^{4+} + \text{H}_2/\text{CO}
\]

Standard electrode potentials:

\[
\text{Cu}^{2+} + 2e^- \rightarrow \text{Cu}^0 \quad E^0 = 0.34\text{V}
\]
\[
\text{Cu}^{2+} + e^- \rightarrow \text{Cu}^{1+} \quad E^0 = 0.15\text{V}
\]
\[
\text{Ce}^{4+} + e^- \rightarrow \text{Ce}^{3+} \quad E^0 = 1.44\text{V}
\]

\[
\text{Ce}^{4+} + 0.5\text{Cu}^0 \rightarrow \text{Ce}^{3+} + 0.5\text{Cu}^{2+} \quad E = E_{\text{red}} - E_{\text{ox}} = 1.61\text{V}
\]
P2: Catalyst characterization

- Operando Quick-X ray Absorption Spectroscopy (XAS)
- Temporal Analysis of Products (TAP)
  - Filtering out of diffusion phenomena
  - Identifiablity of reaction networks
  - thermodynamic time invariances for dual kinetic experiments
Progress P2: Catalyst characterization

 Experiment I

- $F_{CO}=1$, $F_{CO2}=0$
- Inert packing
- $d_p = 250 \div 500 \mu m$
- $L_{reactor} = 30 mm$
- $L_{cat} = 1 mm$

 Experiment II

$\left( \frac{\sqrt{\sqrt{\sqrt{}}}}{\sqrt{\sqrt{}}} \right) \left( \frac{\sqrt{\sqrt{}}}{} \right)$
P3: Adsorption on zeolites

• Hydrocarbon adsorption enthalpies and entropies at T > 0K
• Effect of molecular size and of zeolite
• Idem for alcohols
• Ab initio technique: efficient normal mode analysis of zeolites
P3: PMOs as adsorbents

Mercury(II) ion adsorption

Solid acid catalysis


Progress P4: Polymer design

- **Free radical polymerization Microkinetics**
  - Defects in PolyVinylChloride (PVC)
  - Stereoregularity of conjugated polymers
- **Controlled radical polymerization**
  - Atom Transfer Radical Polymerization (ATRP)
    - microkinetics accounting for diffusion
    - MethylMethAcrylate (MMA), isoBornylAcrylate (iBoA), N-isoPropyl vinylamide (NiPAAM) and styrene
    - Initiators for Continuous Activation Regeneration (ICAR): model based optimization
  - Nitroxide mediated polymerization (NMP)
    - Design of optimal procedures for styrene
    - Mini-emulsion
ICAR ATRP

ATRP initiator + ACTIVATOR

$R_{\text{ini}}X + M_i^*L_2X \xrightarrow{k_{a,\text{ini}}} k_{d,\text{ini}}$

$[M]_0 : [R_{\text{ini}}X]_0 = 50$ and $200$

$[A]_0 = 0 \text{ mol L}^{-1}$

$I_2_0 = 0.02 [R_{\text{ini}}X]_0$

$[D]_0 : [R_{\text{ini}}X]_0 = 0.002$

$T_{\text{pol}} = 353 \text{ K}$

$X_0 = 50$ and $200$

$A_0 = 0 \text{ mol L}^{-1}$

$I_2_0 = 0.02 [R_{\text{ini}}X]_0$

$[D]_0 : [R_{\text{ini}}X]_0 = 0.002$

Challenge:
controlled process using ppm level of Cu catalyst
NMP miniemulsion

- Emulsifier
- NMP initiator $R_{ini}X$
- Phenylethyl-SG1

Styrene droplet (nm)

$T_{pol} = 396$ K
$[M]_0 : [R_{ini}X]_0 = 300$
Progress P5: Reactor design

- Gas-solid vortex reactor
  - range of conditions for stable flow
  - cold flow set-up
  - fast pyrolysis of lignocellulosic biomass (in silico)

- Industrial reactor scale
  - steam cracking
  - slurry reactor for Fischer-Tropsch synthesis
  - riser reactor for Fluid Catalytic Cracking

- Transported Probability Density Functions (pdf’s)
- Reactive Mixing Index (REMI)
Gas/Solid Fluidization Reactors

Conventional Fluidized Bed

Riser/Circulating Fluidized Bed

Conventional Rotating Fluidized Bed

Gas/Solid Vortex Reactor

2. http://www.fluidcodes.co.uk/fbed.html
3. adapted from Watano et al., Powder Tech.131 (2003) 250-255

gravitational technologies

centrifugal technologies
Gas/Solid Vortex Reactor (GSVR)

GSVR Characteristics:
- Gas injection induces powder rotation
- Centrifugal forces balance drag forces
- Dense bed
- High radial slip velocity

Tangential gas injection
Rotating solid particles

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M2dcR2 Methusalem Programme: Advisory Board Meeting, June 19 2012
Experimental GSVR Set-up
Example 1: video while feeding solid
CFD calculated solid volume fraction

2D (with gravity), 0.74 kg/s air, 3250 g bed
Example 2: small particles

70 micron FCC particles (5000 FPS)
CFD calculated solid volume fraction

3D, 0.74 kg/s air, 3250 g bed
(iso-surfaces = 0.40 and 0.01 solids volume fraction)
0.6 $m^3/s$ gas flow rate, 0.035 $kg/s$ biomass
Total solids volume fraction

GS-VR: reactive flow

0.6 m$^3$/s gas flow rate, 0.035 kg/s biomass
Char volume fraction

P6: Renewable feedstocks

- Thermochemical conversion microkinetics
  - Alcohols, terpenes, vegetable oil methyl esters
  - Mixtures containing talloil, fractions derived from waste fats and greases
- Catalytic conversion of alcohols
  - Ab initio thermodynamic adsorption data
  - Ab initio kinetic data for methanol to olefins (MTO)
Summary: M2dcR2 at midterm

Platform is established for Multiscale Modeling and design of chemical

• **Reactions:**
  – Thermochemical conversion of both fossil and renewable feeds
  – Heterogeneously catalyzed reactions
  – Radicalar polymerizations

• **Reactors:**
  – Polymerization
  – Gas-solid reactions
Methusalem Programme: Advisory Board Meeting, June 19 2012

M2dcR2 ⇒ Application Domains

UNIVERSITEIT
GENT

Biomass to liquids

Renewables to chemicals

Functional Polymers

Environmental

Methusalem, Ghent, 11 September 2008

http://www.lct.UGent.be
M2dcR2: future research axes

- Reactor design for process intensification
  - GS-Vortex reactor: hot (reactive) flow unit
  - LS-Vortex reactor: cold flow unit
- Design of functional polymers
  - Controlled Radical Polymerization for complex copolymer architectures
  - Heterogeneous polymerization
- Production of bio-based platform chemicals and liquid fuels
  - Pyrolysis
  - Bioethanol oligomerization
CleanChem

Cleantech for sustainable chemical production
Objectives: general

Cleantech processes, products and services enabling to optimize the use of our resources and minimizing its environmental impact.
## CleanChem expertises

### Transition from fossil to renewable resources

<table>
<thead>
<tr>
<th>Expertise</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Biomass conversion</strong></td>
<td>Chemicals and biofuels</td>
</tr>
<tr>
<td><strong>Process intensification</strong></td>
<td>(Micro)-reactors</td>
</tr>
<tr>
<td><strong>Optimization and innovation</strong></td>
<td>High-throughput methodology</td>
</tr>
<tr>
<td><strong>Scale-up</strong></td>
<td>Pilot plants</td>
</tr>
<tr>
<td><strong>Chemical waste stream treatment</strong></td>
<td>Water treatment</td>
</tr>
<tr>
<td><strong>Sustainability assessment</strong></td>
<td>Measurement methods</td>
</tr>
<tr>
<td><strong>Chemicals and biofuels</strong></td>
<td>Methane valorization</td>
</tr>
<tr>
<td><strong>(Micro)-reactors</strong></td>
<td>In silico reactor design</td>
</tr>
<tr>
<td><strong>High-throughput methodology</strong></td>
<td>Catalysis and green chemistry</td>
</tr>
<tr>
<td><strong>Predictive simulations</strong></td>
<td>Gas treatment</td>
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<tr>
<td><strong>In silico reactor design</strong></td>
<td>Eco-efficiency assessment</td>
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<tr>
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<td>Predictive simulations</td>
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<tr>
<td><strong>Process simulation</strong></td>
<td>Process monitoring</td>
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<tr>
<td><strong>CO2 valorization</strong></td>
<td>Sustainability metrics</td>
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<tr>
<td><strong>Process monitoring</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Measurement methods</strong></td>
<td></td>
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</tbody>
</table>
CleanChem scope in UGent

- Chemical technology
- Fossil resources
- Renewables
- (Base) chemicals
- Energy carriers
- White biotechnology
- Ghent Bio-energy Valley
- Polymer reaction engineering
- Polymerization technology
- Chemical technology
- Specialty chemicals
- Chemtech
- Ghent Bio-energy Valley
- M2dcR2 Methusaleum Programme: Advisory Board Meeting, June 19, 2012
M2dcR2 Methusalem Programme: Advisory Board Meeting, June 19 2012

CleanChem organogram

**CleanChem**

**steering committee**

**FIRW**
**FBW**
**WE**
**Associatie**

- **IOF mandatory**
  - valorization management

- **Guy Marin**
  - chemical reactor and reaction engineering

**Wolter Prins**
- biomass conversion

**Geraldine Heynderickx**
- reactor engineering/hydrodynamics

**Joris Thibaut**
- catalytic reaction engineering

**Kevin Van Geem**
- thermochemical processes / pilot / feedstock analysis

**Ingmar Nopens**
- waste treatment: modeling

**Jo Dewulf**
- clean tech and sustainability assessment

**Eveline Volcke**
- biosystems control

**Stijn Van Hulle**
- water treatment and environmental engineering

**Jeriffa De Clercq**
- scale-up catalyst synthesis/water treatment

**Pascal Van Der Voort**
- ordered mesoporous catalysts

**Marie-Françoise Reyniers**
- ab-initio reaction kinetics and polymer reaction engineering

**Chris Stevens**
- green chemistry/renewables/microreactors

**Isabel Van Driessche**
- sol gel catalyst synthesis

**Vladimir Galvita**
- catalytic reaction kinetics: experimental techniques
<table>
<thead>
<tr>
<th>Project Description</th>
<th>Start</th>
<th>End</th>
<th>Budget (k€)</th>
<th>Principal Investigator(s)</th>
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<tr>
<td>Oxidative Coupling of Methane followed by Oligomerization to Liquids (OCMOL; coordinator; EC-FP7)</td>
<td>2009</td>
<td>2014</td>
<td>830</td>
<td>Marin/Thybaut</td>
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<td>Innovative Catalytic Technologies &amp; Materials for Next Gas to Liquid Processes (NEXT-GTL; EC-FP7)</td>
<td>2009</td>
<td>2013</td>
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<td>Thybaut</td>
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<td>Multiscale Modeling of Chemical and Biochemical Systems (MULTIMOD; EC-FP7)</td>
<td>2009</td>
<td>2013</td>
<td>310</td>
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<td>Fouling in the convection section tubes of a steam cracker (FWO)</td>
<td>2009</td>
<td>2012</td>
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<td>Coking Sensitivity II (company)</td>
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<td>Steam Cracking (company)</td>
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<td>Meerschalige studie van reactieve gasinjectie in pyrometallurgische processen (FWO)</td>
<td>2010</td>
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<td>Multiscale modeling of aromatics hydrogenation (research institute)</td>
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<td>Kinetic Modelling of Fischer-Tropsch Synthesis</td>
<td>2010</td>
<td>2015</td>
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<td>Atomic Layer Deposition (ALD): a new tool for model based tailoring of acid catalytic activity</td>
<td>2011</td>
<td>2014</td>
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<td>In situ XAS study of ALD of bimetallic materials</td>
<td>2011</td>
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<td>Functional Supramolecular Systems (IUAP VII;BELSPO)</td>
<td>2012</td>
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<td>Multiscale Analysis and Design for Process Intensification and Innovation (MadPIL; EC-FP7)</td>
<td>2012</td>
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<td>Model-based Optimization &amp; Control for Process-Intensification and Biopharmaceutical Systems (OPTICO)</td>
<td>2012</td>
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<td>Production of Clean Fuels and Chemicals by fast Pyrolysis of Lignocellulosic Biomass (BIO-OIL ;BOF-UGent)</td>
<td>2012</td>
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<td>Intrinsic Catalytic Kinetics Anamized and Reconciled with Industrial Conditions (ICKARUS; EC-FP7-PEOPLE)</td>
<td>2012</td>
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<td>Ontwikkeling van multi-stap synthesesequenties voor functionele polymeermaterialen door combinatie van één-potprocedures en model gestuurd ontwerp (DOMINO-CLICK; FWO)</td>
<td>2012</td>
<td>2015</td>
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<td>Koolstof-adsorbentia- Rationeel ontwerp van mesoporeuze koolstof-adsorbentia voor de verwijdering van organische polluenten uit water ( OF-Associatie) UGent)</td>
<td>2012</td>
<td>2016</td>
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<td>Development of highly selective and stable adsorbents for removal and recycling of rare earths (Associatie-UGent)</td>
<td>2012</td>
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<td>13h45</td>
<td>P1 “Biomass to Olefins: Steam Cracking of Renewable Feedstocks ” by Steven Pyl</td>
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<td>P2-P3 “the catalytic performance of Vanadium based Metal Organic Frameworks in the oxidation of cyclohexene ” by Karen Leus</td>
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<td>P5 “Multi-scale modeling and reaction path analysis of benzene hydrogenation on Pd(111) “ by Gonzalo Canduela</td>
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<td>P6 “Application of microreactor technology for the modification of renewable resources “ by Ana Cukalovic</td>
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General discussion

• strengths?
• weaknesses?
• opportunities?
• threats?
• research priorities
• equipment
Next advisory board meeting

• date

• format

• reporting/minutes of meeting
Defended PhD theses in 2012

- The Thermochemistry and Decomposition Mechanism of Organosulfur and Organophosphorus Compounds
  Aäron Vandeputte
  Advisors: Marin, G.B.; Reyniers, M.-F.
  January 2012

- Hydrogenation of Aromatics: Single-Event Microkinetic (SEMK) Methodology and Scale-Up
  Tapan Bera
  Advisors: Marin, G.B.; Thybaut, J.W.
  March 2012
Defended PhD theses in 2011

- Modeling of Reaction, Attrition and Breakage in Gas-Solid Multiphase Flow Systems Using the Quadrature Method Approach
  Abhishek Dutta
  Advisors: Constales, D.; Heynderickx, G.J.
  January 2011

- Mathematical determination of reaction networks from transient kinetic experiments
  Raf Roelant
  Advisors: Constales, D.; Marin, G.B.
  January 2011

- The total oxidation of propane over metal oxide catalysts: transient kinetics and monolith reactors
  Veerle Balcaen
  Advisors: Marin, G.B.
  February 2011

- Single-Event Microkinetics of Hydrocarbon Cracking on Zeotype Catalysts: Effect of Acidity and Shape Selectivity
  Rhona Van Borm
  Advisors: Marin, G.B.; Reyniers, M.-F.
  February 2011
Defended PhD theses in 2011

  Bart De Moor
  Advisors: Marin, G.B.; Reyniers, M.-F.
  February 2011
Defended Ph D theses in 2010

- Modeling of gas-solid reactive flow using a hybrid finite volume and probability density function method
  *Suryanarayana Prasad Vegendla*
  Advisors: G.J. Heynderickx and G.B. Marin
  January, 2010

- Kinetic Modeling of Atom Transfer Radical Polymerization of (Meth)acrylates
  *Dagmar R. D’hooge*
  Advisors: G. B. Marin and M.-F. Reyniers
  May, 2010
## Joint publications

### 2009

<table>
<thead>
<tr>
<th>Title</th>
<th>Authors</th>
<th>Journal</th>
<th>Volume, Issue, Pages</th>
<th>Year</th>
<th>SCI-IF (2008)</th>
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### Joint publications

**2009**


Microkinetic modelling of structural properties of poly(vinyl chloride)  
J. Wieme, M.-F. Reyniers, G.B. Marin  

Synergy between shape selective and non shape selective bifunctional zeolites modeled via the Single-Event MicroKinetic (SEMK) methodology  

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### 2010

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<tr>
<td>Initiator efficiency modeling for vinyl chloride suspension polymerization</td>
<td>J. Wieme, M.-F. Reyniers, G.B. Marin</td>
<td>Chemical Engineering Journal</td>
<td>154</td>
<td>203-210</td>
<td>2010</td>
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<td>Steady-state simulation of Fluid Catalytic Cracking riser reactors using a decoupled solution method with feedback of the cracking reactions on the flow</td>
<td>E. Baudrez, G.J. Heynderickx, G.B. Marin</td>
<td>Chemical Engineering Research and Design</td>
<td>88</td>
<td>290-303</td>
<td>2010</td>
<td>1.223</td>
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<tr>
<td>Catalytic cracking of methylcyclohexane on FAU, MFI, and bimodal porous materials: influence of acid properties and pore topology</td>
<td>R. Van Borm, M.-F. Reyniers, J.A. Martens, G.B. Marin</td>
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<td>Modeling the coke formation in the convection section tubes of a steam cracker</td>
<td>S.C.K. De Schepper, G.J. Heynderickx, G.B. Marin</td>
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<td>Micromixing effects on Series-Parallel and Autocatalytic Reactions in a Turbulent Single-Phase Gas Flow</td>
<td>S.N.P. Vegendla, G.J. Heynderickx, G.B. Marin</td>
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<td>Theoretical study of the adsorption of C1-C4 primary alcohols in H-ZSM-5</td>
<td>C.M. Nguyen, M.-F. Reyniers, G.B. Marin</td>
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## 2010

**Atom Transfer Radical Polymerization of Isobornyl Acrylate: a Kinetic Modeling Study**  


**Molecular reconstruction of complex hydrocarbon mixtures: an application of principal component analysis, S.P. Pyl, K.M. Van Geem, M.-F. Reyniers, G.B. Marin**  

**Online analysis of complex hydrocarbon mixtures using comprehensive 2D gas chromatography, K.M. Van Geem, S.P. Pyl, M.-F. Reyniers, J. Vercammen, J. Beens, G.B. Marin**  

**Accurate High-Temperature Reaction Networks for Alternative Fuels: Butanol Isomers**  
2010

### Joint publications

**2011**

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<tr>
<td>First Principle-Based Simulation of Ethane Steam Cracking</td>
<td>Sabbe, M.K.; Van Geem, K.M.; Reyniers, M.-F.; Marin, G.B.</td>
<td>AlChE Journal</td>
<td>57, 2, 482-496</td>
<td>2011</td>
<td>2.030</td>
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<td>Reciprocal relations between kinetic curves</td>
<td>Yablonsky, G.S.; Gorban, A.N.; Constales, D.; Galvita, V.V.; Marin, G.B.</td>
<td>EPL - Europhysics Letters</td>
<td>93, 2, 20004</td>
<td>2011</td>
<td>2.753</td>
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<td>Methane</td>
<td>Marin, G.B.</td>
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<td>Adsorption of C2-C8 n-Alkanes in Zeolites</td>
<td>Waroquier, M.; Marin, G.B.</td>
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**2011**

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<td>Reaction network for the total oxidation of toluene over CuO-CeO2/Al2O3</td>
<td>Menon, U.; Galvita, V.V.; Marin, G.B.</td>
<td><em>Journal of Catalysis</em></td>
<td>283, 1, 1-9</td>
<td>2011</td>
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**2011**

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### 2011


## 2012

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<tr>
<td>**Thermodynamic time invariances for dual kinetic experiments: nonlinear single</td>
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<td>reactions and more**, Constales, D.; Yablonsky, G.S.; Marin, G.B., Chemical</td>
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<td>The coordinatively saturated vanadium MIL-47 as a low leaching heterogeneous</td>
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<td>catalyst in the oxidation of cyclohexene, Leus, K.; Vandichel, M.; Liu, Y.-Y.;</td>
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<td>Muylaert, I.; Musschoot, J.; Pyl, S.P.; Vrielinck, H.; callens, F.; Marin, G.B.;</td>
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<td>Detavernier, C.; Wiper, P.V.; Khimyak, Y. Z.; Waroquier, M.; Van Speybroeck, V.;</td>
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<td>Kinetic modeling of ICAR ATRP, D’hooge, D.R.; Konkolewicz, D.; Reyniers, M.-F.;</td>
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<td>Marin, G.B.; Matyjaszewski, K., Macromolecular Theory and Simulations, 21, 52-69,</td>
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<td>Kinetic Modeling of Miniemulsion Nitroxide Mediated Polymerization of Styrene:</td>
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<td>Effect of Particle Diameter and Nitroxide Partitioning up to High Conversion,</td>
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<td>Bentein, L.; D’hooge, D.R.; Reyniers, M.-F.; Marin, G.B., Polymer, 53, 681-693,</td>
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**2012**

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M2dcR2 ⇒ Applications-FP7

- FP7-ITN-4selox-Highly Selective Catalysts for Alkene Oxidation through Fundamental Understanding (aanvraag jan. 2012)

- FP7-PEOPLE-Biolefins-Lignocellulosic Biomass Conversion for the Production of Light Olefins (aanvraag april 2012)
  G.B. Marin, M. Ruitenbeek, F. Van Damme
IWT-OLEON-Duurzame productie van propyleenglycol uit glycerine
(aanvraag febr. 2012)

G.B. Marin, J.Thybaut, D. Packet
FWO-JoKiREx-Joint kinetics of reciprocal experiments (aanvraag maart 2012)
   G.B. Marin, D. Constales

FWO-XAS-TEM-Modified iron oxide materials for hydrogen production studied by operando XAS and TEM (aanvraag maart 2012)
   G.B. Marin, H. Poelman, G. Van Tendeloo

FWO-MULTISCALECRP-First principles based multi-scale modeling of controlled radical polymerisation processes (aanvraag maart 2012)
   M.-F. Reyniers, G. Heynderickx

FWO-Micro-Pyro- Pyrolysis of organic waste streams, activation and regeneration of activated carbon using microwave heating (aanvraag maart 2012)
   J. Yperman, R. Carleer, K. Van Geem

FWO-PMO-BZBK- Periodic Mesoporous Organosilica (PMO) as bifunctional acid/base catalysts (aanvraag april 2012)
   P. Van Der Voort, P. Cool, J. Thybaut
M2dcR2 ⇒ Applications not honoured in 2010-SBO

- **SBO: Promicro**-Process Intensification by Integrated Microreactor Technology for the Chemicals using Industry

- **SBO:INCA**-Rational Design of Industrial Catalysts
  J. Paul, G. Huyberechts, P. Van Der Voort, J. Thybaut, A. Verberckmoes, J. De Clercq, B. Sels
Applications not honoured in 2010-MPR

- MPR-Multidisciplinary Research Partnerships-Functional Nanomaterials for Sustainable Chemistry and Energy conversions

  V. Van Speybroeck, M. Waroquier, G.B. Marin, C. Detavernier, P. Van Der Voort, F. Du Prez, B. Clarysse
Applications not honoured in 2010-GOA

- **GOA-PYROKIN**: Pyrolysis Kinetics: Optimization of biomass and bio-oil composition for sustainable and renewable production of energy carriers, biofuels and chemicals

M2dcR2 ⇒ Applications not honoured in 2011-FP7

- **FP7-ITN-4selox-Highly Selective Catalysts for Alkene Oxidation through Fundamental Understanding**

- **FP7-PICULA-Development of a fully integrated process for the decentralized production of stabilised pyrolysis oil from sustainable biomass**

- **FP7-SUCHARA-Solutions for Utilizing CarboHydrates As Renewable Alternatives**
Applications not honoured in 2011-ERC

- ERC- Starter Grant - *CatBiChem*-Model Guided Design of the Catalytic Transformation of Biomass into Fuels and Chemicals
  
  J. Thybaut
Applications not honoured in 2011-FWO

- **FWO-MICROREACTOREN** - Experimental and computational study of microreactor technology for reactions with diazomethane
  
  G. Heynderickx, C. Stevens

- **FWO-FCC-proces** - Experimental and computational analysis of particle behavior in the FCC process
  
  G. Heynderickx, I. Nopens

- **FWO-Project** - Periodic Mesoporous Organosilica (PMO) as bifunctional acid/base catalysts
  
  P. Van Der Voort, P. Cool, J. Thybaut

- **FWO-Time-resolved operando XAS and TEM study of the promoter effect in modified iron oxide materials for hydrogen production**
  
  G.B. Marin, L. Kestens, K. Verbeken, H. Poelman
Applications not honoured in 2012-FP7

- **FP7-**UPLIFT-Ultra Performance Low Impact Fischer-Tropsch
  

- **FP7-**CIROP-Catalysis In Renewable Oil Production
  
  D. Farrusseng, G. Marin; M.-F. Reyniers; E. Tsang; E Shotton, Anna kroner, S. Ellis, P. Ellis, G. Kelly; D. James, C. Thieuleux, A. Quadrelli, Y. Schuurman, C. Mirodatos, J.-L. Rousset
M2dcR2 ⇒ Applications not honoured in 2012-IWT

- IWT-SBO-BIOLEUM-Fuels and chemicals by fast pyrolysis of biomass
  G.B. Marin, W. Boerjan, J. Van Acker, W. Prins
M2dcR2 ⇒ Applications not honoured in 2012-BOF

- BOF-GOA-SoHy-Solar Hydrogen: fueling the future
  D. Poelman, I. Van Driessche, J. Thybaut, A. Adriaens, H. Poelman, K. De Buyssser, P. Lommens

- BOF-GOA-ALiBi-Compositional Analysis of Lignocellulosic Bio

- BOF-GOA-COMPABAR-Computational study of particle attrition, breakage and aggregation in gas-solid two-phase flow reactors
  G. Heynderickx, I. Nopens