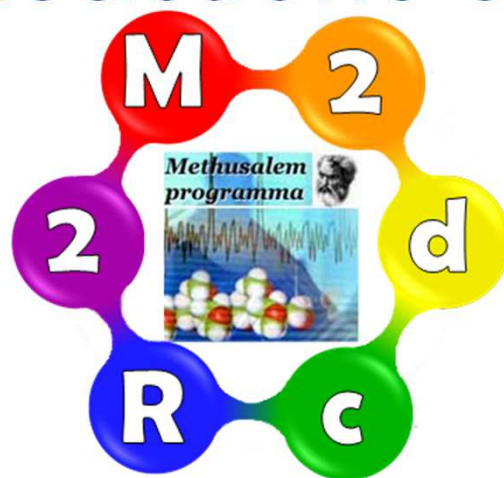


Multi-scale Modeling and design of chemical Reactions and Reactors



Guy B. Marin



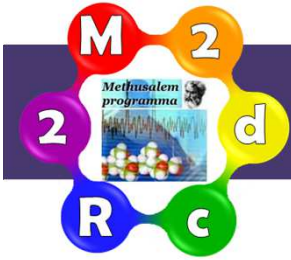
Agenda Annual Meeting IAB

- 8 h 45: Welcome/ Coffee
- 9 h 00: Minutes/Excused (Sautet,Barner-Kowollik,Weckhuysen,Stevens,Saeys)/Introduction
- 9 h 10: Minutes meeting 19/06/2014 (sent on 18/07/2014)
- 9 h 20 : **Axis 1a**: Platform for design of functional materials: polymers by Dagmar D'hooge
- 9 h 50 : **Axis 1b**: Platform for design of functional materials: catalysts by Vladimir Galvita
- 10 h 20: Break
- 10 h 30: **Axis 2**: Reactor design for process intensification by Geraldine Heynderickx
- 11 h 00: **Axis 3**: From Fossil to renewable feedstocks: Hans-Heinrich Carstensen
- 11 h 30: First term evaluation procedure and second term proposal procedure Guy B. Marin



Agenda Annual Meeting IAB

- 12 h 00: Posters intro 2 minutes each
- 12 h 30: Lunch/Poster session
- 14 h 00 : Summary of the final report of the first term of the programme by Guy B. Marin
- 14 h 30 : Presentation of the proposal for the second term by Maarten Sabbe and Paul Van Steenberge
- 15 h 00 : Discussion
- **15 h 45** : Deliberation of IAB based on received report and presentations
- 16 h 30 : Feedback by IAB to MC members
- 17 h 00 : End of meeting



Methusalem program: general

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”



Aim : world top centre at UGent

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

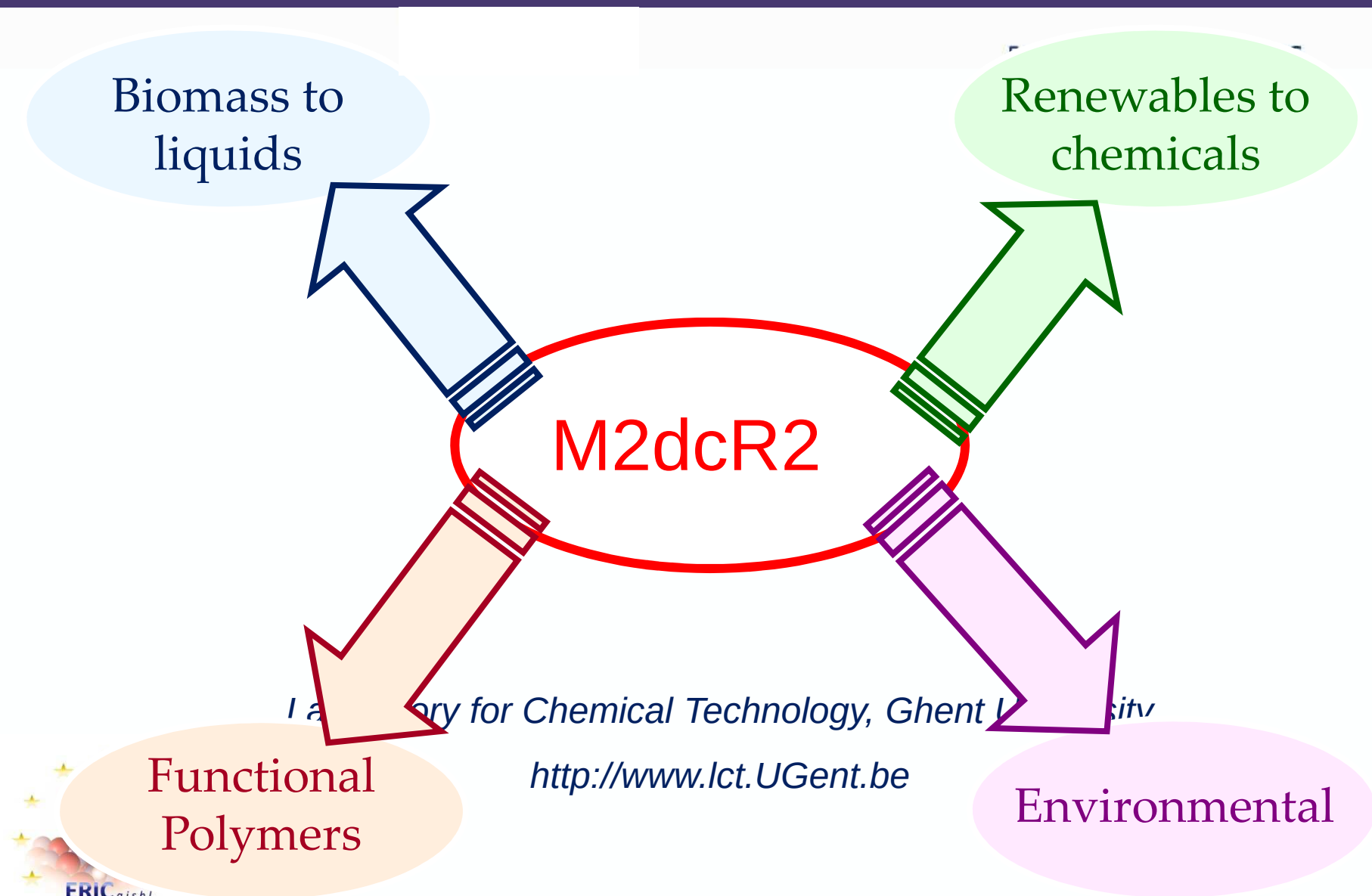
Methusalem proposal presentation, 11 September 2008



Subprogrammes

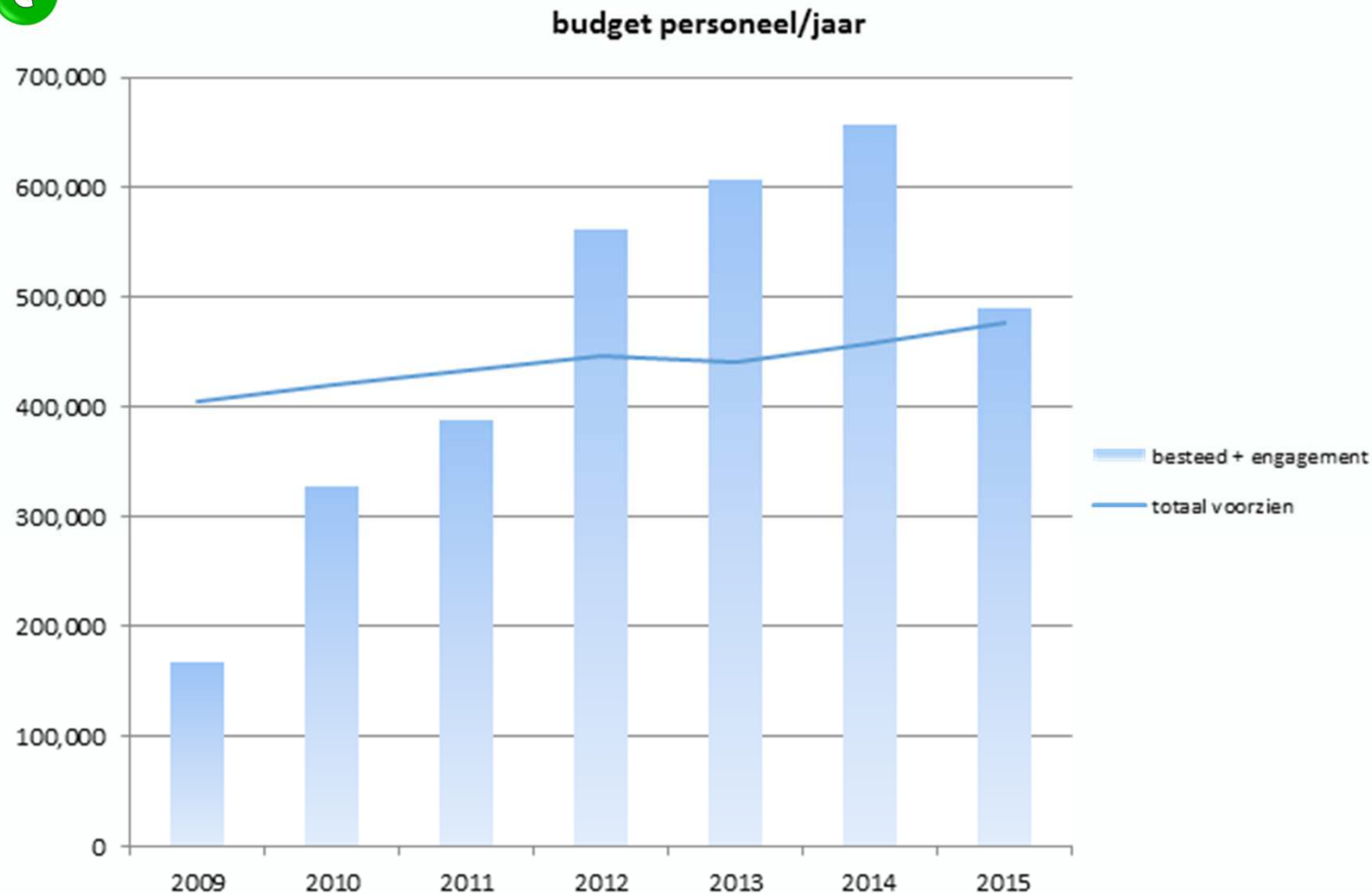
	subprogramme	MC member
P1	Single event microkinetics (SEMK) in complex reaction mixtures	J. Thybaut, M.-F. Reyniers, K. Van Geem, M. Sabbe
P2	Catalyst design based on catalyst descriptors	J. Thybaut, M.-F. Reyniers, P. Van der Voort, M. Saeys, M. Sabbe
P3	Adsorption by nanoporous materials	J. Thybaut, M.-F. Reyniers, M. Saeys
P4	Polymer design accounting for diffusion and mixing	G. Heynderickx, M.-F. Reyniers, D. D'Hooge
P5	Reactor design from first principles	G. Heynderickx, K. Van Geem, D. Constaes, M. Sabbe
P6	From fossil to renewable feedstocks	C. Stevens, J. Thybaut, M.-F. Reyniers, K. Van Geem

M2dcR2 $\Rightarrow$ Application Domains





Budget and spending for researchers



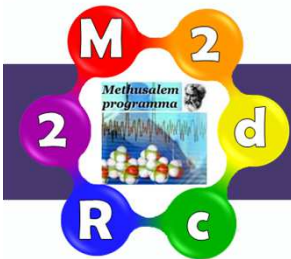
June 9 2015



Unique infrastructure

- High throughput units for kinetics





Unique infrastructure

- Temporal Analysis of Products (TAP)





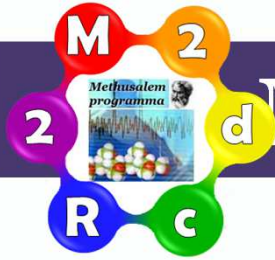
Ex post evaluation

- Quality of work
- Human resources management
- Research plan for next term
- Negative evaluation/resigning of PI
 - yearly reduction with 25%

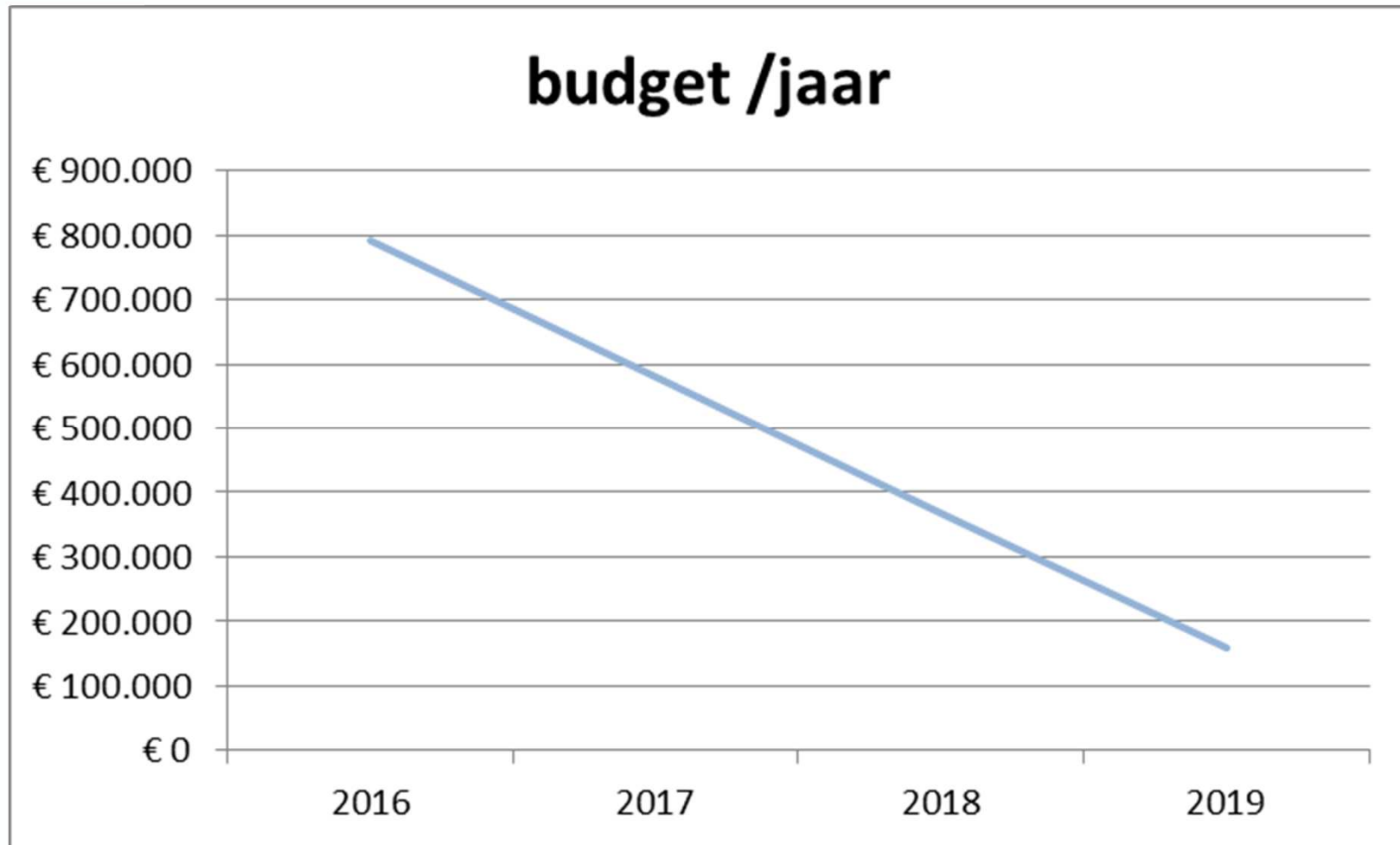


Mails dd 24/04/2014 and 02/04/2015

- Mails dd 22/04/2014 and 02/04/2015 :
 1. No evaluation by external panel
 2. Research Council of Ghent University has to agree with the budget for the second term reduced according to the prescribed rules



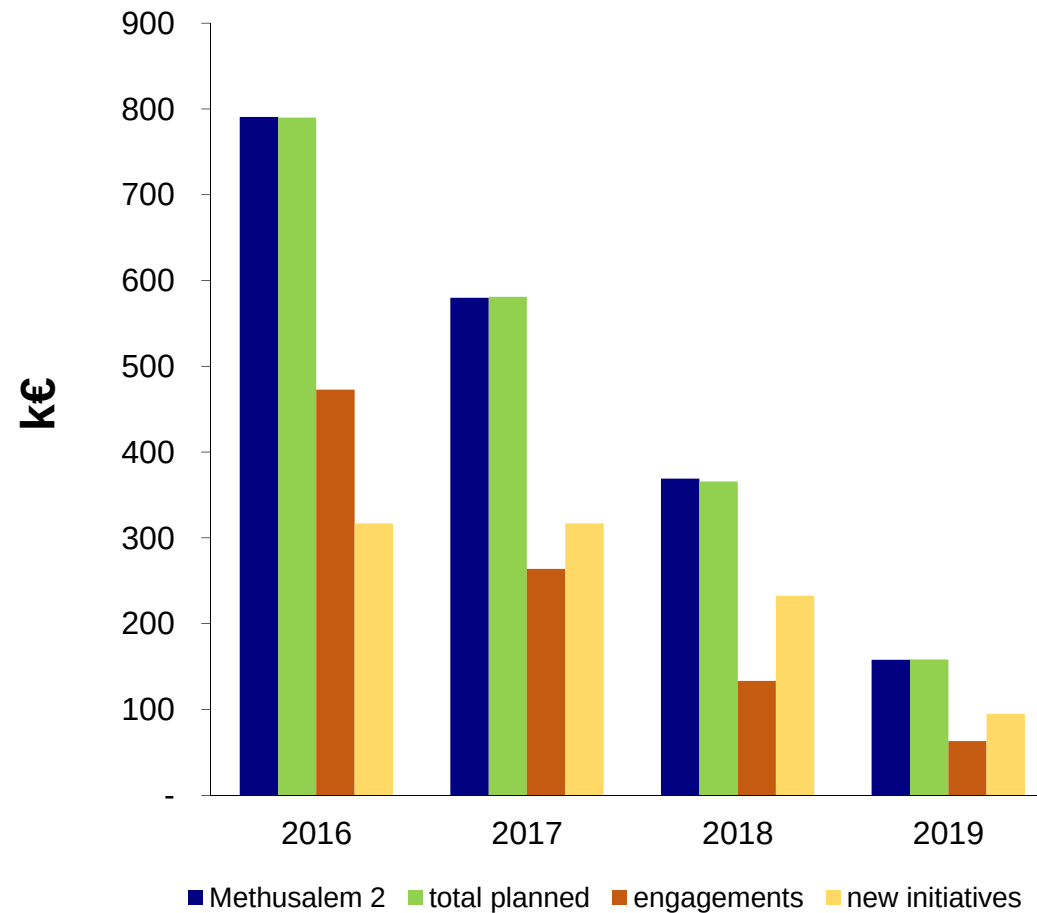
Mails dd 24/04/2014 and 02/04/2015



1.897.714 €

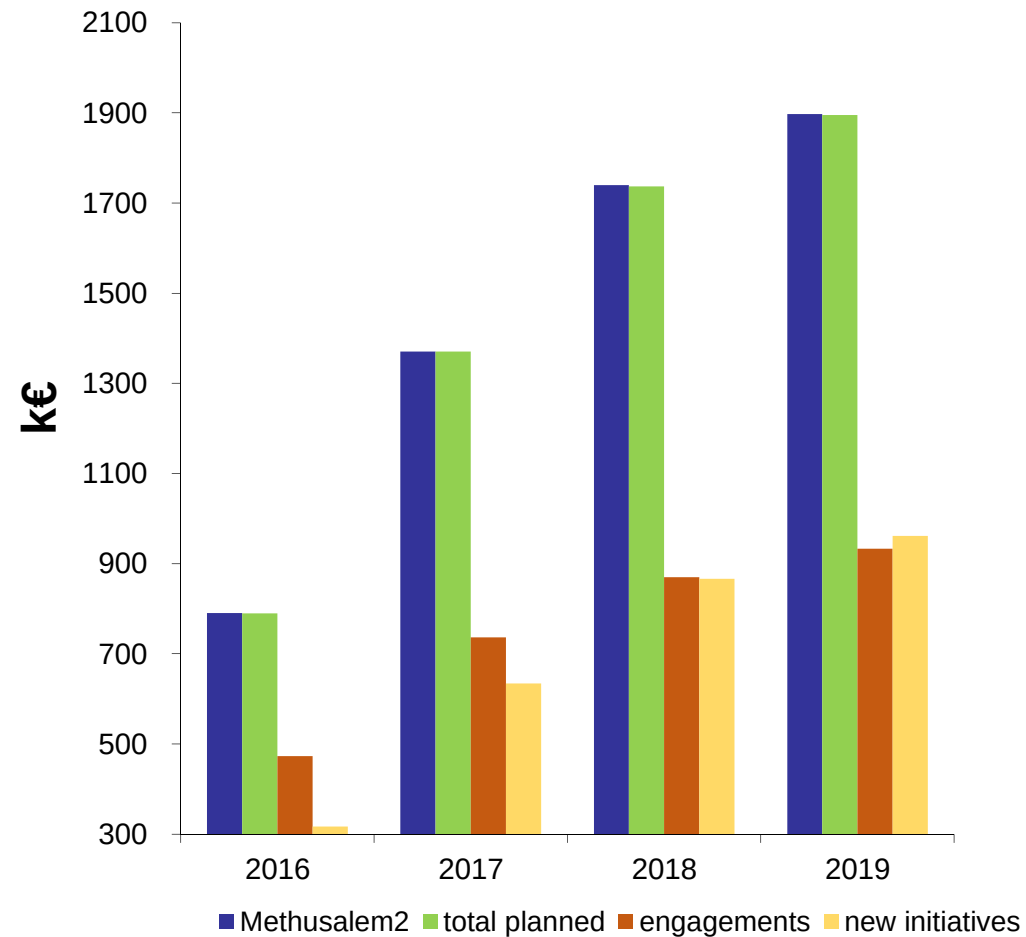


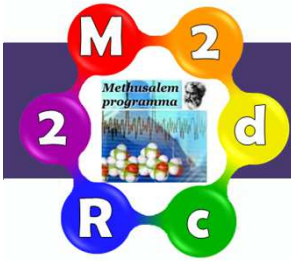
Budget breakdown





Cumulative budget breakdown





Post 2015: evaluation

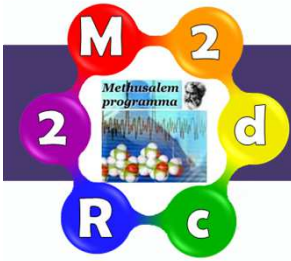
1. Oorspronkelijk gestelde doelstellingen
2. Maximum 10 bullets with achievements
3. Explanation of achievements (6-10 pages)
4. 10 publications with brief explanation
5. PhD's defended (2009-Aug. 2015)
 1. Within scope of M2dcR2: 46
 2. Out of scope: 9
6. PhD's in preparation
 1. Within scope of M2dcR2: 62
 2. Out of scope: 15



Midterm Review by IAB

1. Scope

- methods for kinetic and reactor modeling
- combination of ab initio, microkinetics and reactor models
- growth of materials by first principles
- macromolecular reaction engineering



Midterm Review by IAB

2. Input factors

- teams well staffed
- collaboration between members now adequate
- attention to maintain scientific staffing required
- investments and expenses adequate



Midterm Review by IAB

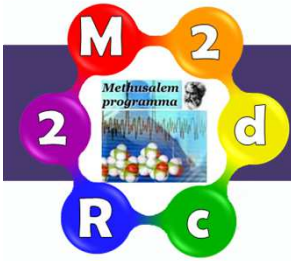
3. Results and recommendations (1/3)

- impressive amount of high level PhD theses
- vast amounts of high fidelity scientific data
- number and quality of publications very good (239 joint publications as of today)
- at least one high profile publication in journal such as Nature asked for



High impact papers

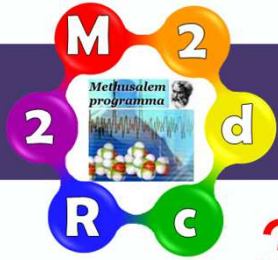
1. Experimental and Theoretical Methods in Kinetic Studies of Heterogeneously Catalyzed Reactions, *M.-F. Reyniers, G.B. Marin, **Annu. Rev. Chem. Biomol. Eng.** 5, 563-594, 2014*
SCI-IF: 8.109 (2013)
2. A state-of-the-art review on the potential of kinetic modeling to optimize CRP processes in homogeneous and heterogeneous medium, *D.R. D'hooge, P.H.M. Van Steenberge, M.-F. Reyniers, G.B. Marin, **Prog. Polym. Sci.***
(invited and submitted); SCI-IF: 26.845 (2013)
3. Origin of Extraordinary Stability of Square Planar Carbon in Surface Carbides of Co and Ni, and Beyond, A. Nandula, Q.T. Trinh, M. Saeys, A.N. Alexandrova, **Angew. Chem. Int. Ed., VIP paper, 2015**, 54 (18), 5312–5316, SCI-IF: 11.336 (2013)



Midterm Review by IAB

3. Results and recommendations (2/3)

- good level of CFD work, combination with chemical kinetics required
- use of open-source CFD codes such as OpenFOAM recommended



Midterm Review by IAB

3. Results and recommendations (3/3)

- impressive activity of submitting new projects
- impressive seeding towards full-fledged new projects
- attention to be paid to the focus of this already pretty broad program
- attention for heterogeneous target audience required
- branding of program as one entity required



E.Lox 26/07/2013

- timeline PhD projects (comment 1)
 - see slides and appendix of progress report
- website (comment 5)
- societal impact/industrial roadmaps (comment 4,6-9)
 - CleanChem
 - Sustainable Chemistry in Ghent
- branding concept (comments 2 and 3)
 - FORTE (LCT; quotation 05/05/15)



10 bullets with achievements

Axis 1 Platform for design of polymers

1. Experimental determination of termination rate coefficients
2. Bivariate description of copolymer microstructure

Axis 1 Platform for design of catalysts

1. Integrated Stefan-Maxwell, Mean Field Approximation and Single-Event MicroKinetic (SEMK) models
2. Design of cooperative acid-base catalysts for aldol condensation
3. Validation and application of ab initio based microkinetic model for bio-ethanol dehydration to ethene



10 bullets with achievements

Axis 2 Reactor design for process intensification

1. 3D reactor technology for intensified heat transfer
2. Vortex reactor technology for biomass pyrolysis

Axis 3 Transition from fossil to renewable feedstocks

1. Thermal conversion of oxygenates to light olefins
2. GCxGC analysis of bio-oils
3. Synthetic pathways for sophorolipid based salts with antimicrobial activity



Axis 1 Platform for design of polymers

Axis 1 Platform for design of functional materials: Functional polymers																				
Project		12				13				14					15			Position	Funding	P
Multi-scale modeling of radical polymerization (code development: Monte Carlo; heterogeneous)	Paul Van Steenberge																	NTT AP	UGent	1,4
Multi-scale modeling of RAFT polymerization: homopolymerization and diffusional limitations	Pieter Derboven																	PhD	IWT	4
NMP microkinetics: ab initio LFER	Cuong Manh Nguyen																	Postdoc	FWO	1,4
NMP microkinetics: homogeneous	Stijn Fierens																	PhD	FP7 OPTICO	4
RAFT microkinetics: heterogeneous	Dries Devlaminck																	PhD	IAP	4
Amine-thiol-ene click + Microkinetics RAFT polymerization: ab initio LFER	Gilles Desmet																	PhD	FWO	4
RAFT polymerization microkinetics: experimental: homo- & copolymerization	Nils De Rybel																	PhD	FWO	4
PSD and CLD control in polymerization	Yoshi Mariën																	PhD	M2dcR2/IWT	4
CRP microkinetics: branched and network polymers	Lies De Keer																	PhD	M2dcR2/IWT	4
Reactive extrusion: kinetic modeling and optimization	Julio Ortiz																	Postdoc	Company	4



Axis 1 Platform for design of catalysts

Axis 1 Platform for design of functional materials: Catalysts																				
Project		12				13				14				15				Position	Funding	P
Joint kinetics of reciprocal experiments	Daniel Branco Pinto																	PhD	UGent-BOF	2,3
Intrinsic Catalytic Kinetics Analyzed and Reconciled with Industrial Conditions (ICKARUS)	Evgenyi Redekop																	Postdoc	FP7 MC/M2dcR2	2
In situ synthesis of Au and TiO2 nanoparticles anchored in the framework of functionalized MOF's: selective oxidations	Karen Leus																	Postdoc	UGent-BOF	2
Functionalized Periodic Mesoporous Organosilicas: Superacids and Nanoparticles	Dolores Esquivel																	Postdoc	FWO	2
Development of (Al,V) Bi-Metallo Organic Frames (MOF's) – In situ study of their behavior as catalyst and adsorbent	Hannes Depauw																	PhD	FWO	2,3
Development of highly selective and stable adsorbents for removal and recycling of rare earths	Jeroen De Decker																	PhD	UGent-BOF	3
Rational design of mesoporous carbon adsorbents for removal of organic components from water	Wannes Libbrecht																	PhD	UGent-BOF	3
Periodic Mesoporous Organosilica (PMO) as bifunctional acid/base catalysts	Sander Clerick																	PhD	FWO	2
Rational Catalyst Design for Tar Reforming: A Kinetics Driven Methodology	Stavros Theofanidis																	PhD	FP7 FASTCARD	2
A Multi-Scale Modelling Platform aiming at Rational Catalyst Design for Catalytic Cracking	Roxanne Hubesch																	PhD	FP7FASTCARD	2
A Multi-Scale Modelling Platform applied towards Fischer Tropsch Synthesis on Fe catalysts	José Rivera de la Cruz																	PhD	FP7 FASTCARD	2
Design methodology for hydrodeoxygenation of fast pyrolysis oil	Chanakya Ranga																	PhD	IWT-Bioleum	2
Catalyst Design for Fast Pyrolysis Oil Hydrodeoxygenation	Daria Otyuskaya																	PHD	FP7 FASTCARD	2
Kinetics and design of bimetallic catalysts	Stephanie Saerens																	PhD	Ugent	2
In situ XRF and XAS study of Atomic Layer Deposition (ALD)- deposition of bimetallic materials	Matthias Filez																	PhD	FWO	2
A generic methodology for the microkinetic assessment of catalytic reaction kinetics	Naghmeh Fatemi																	PhD	ERC i-CaD	1,2
Development of a VOx/WOx-catalyst on mesoporous titania for the Oxidative Dehydrogenation of propane	Isabelle Ascoop																	PhD	M2dcR2	2
Fischer-Tropsch synthesis and catalyst design	Kasun Gunasooriya																	Phd	FWO-Odysseus	2
Single-Event MicroKinetic (SEMK) modelling of complex reaction networks	Simon Pressinger																	PhD	FP7 i-CaD	2,5
Optimizing cooperative catalysis in aldol condensation	Jeroen Lauwaert																	Phd	M2dcR2	2
Catalyst optimization for glycerol hydrogenolysis	Alexandra Bouriakova																	PhD	ERC i-CaD	2
Modeling-guided design of selective catalysts. Effect of boron promotion	Ruijin Hou																	Postdoc	FWO-Odysseus	2
Modeling guided design of selective catalysts.	Gerard Novell-Leruth																	Postdoc	FWO-Odysseus	2



Axis 2 Reactor design for process intensification

Axis 2 Reactor design for process intensification																
Project		12			13			14			15			Position	Funding	P
(Reactive) powder flow	Maria Pantzali													NTT AP	UGent	5
Fast biomass pyrolysis in RFB-SG	Hans-H. Carstensen													senior scientist	ERC-MADP II	5,6
Gas-solid heat & mass transfer	Max Friedl													PhD	ERC-MADP II	5
Riser and vortex flow (cold flow)	Maria del Mar Torregrosa													Postdoc	ERC-MADP II	4,5
Reactive powder flow: biomass (literature based kinetics)	Ana Obradovic													Postdoc	ERC-MADP II	5,6
CFD modeling cold & reactive flow	Kaustav Niyogi													PhD	ERC-MADP II	5
New reactor geometries for pyrolysis	David Van Cauwenberge													PhD	Baekeland	5
Fouling in Evaporators	Pieter Verhees													PhD	Company	5
Reactor material selection for fouling mitigation	Stamatis Sarris													PhD	Company	5
Fouling mitigation by additives	Natalia Olahova													PhD	Company	5
Short contact time partial oxidation of methane	Songjun Liu													PhD	ERC-MADP II	5
Fouling in heat Exchangers	Nenad Ristic													PhD	Company	5
Micro- and millireactor technology for batch reactions difficult to scale up	Frederik Van Waes													PhD	FWO	5
Mesoporous silicas and zeolites as heterogenous catalyst for micro- and millireactor technology	Sofie Seghers													PhD	UGent-BOF	5
Photochemistry in microreactors	Thomas Heugebaert													Postdoc	FWO	5
Development of a chemical heat pump to valorize rest heat	Matteo Ciprian													junior scientist	Company	5
Design and demonstration of reactive Gas Solid Vortex Reactor	Arturo Gonzales Quiroga													PhD	Bioleum/MADP II	5,6
Reactor simulation from first principles: Fischer Tropsch synthesis	Jonas Van Belleghem													PhD	FWO	2,5
Applying detailed kinetics of hydrotreating and Fischer Tropsch to large-scale reactor simulation	Luis Lozano													PhD	Company	2,5
Modeling of furnaces for endothermic reactions	Yu Zhang													Phd	M2dcR2	5
Process intensification through reactive flow modulation	Jens Dedeyne													PhD	FWO-PiFlow	5
Multiscale modeling of carbon deposition: from carbon nanotube whiskers to free radical coke formation	Alexander Vervust													PhD	FWO/BOF	5
Development of a center of expertise and pilot production installation for industrial flow processes in Flanders	Mathias Moens													Postdoc	FISCH-ICON	4



Axis 3 Transition from fossil to renewable feedstocks

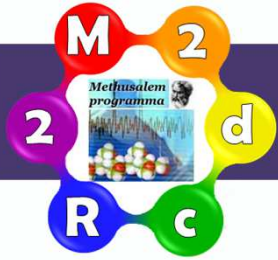
Axis 3 Transition from fossil to renewable feedstocks																
Project		12			13			14			15			Position	Funding	P
MD of acid catalyzed conversion of bio-alcohols	Kostas Alexopoulos													NTT AP	UGent	1,2,3,6
Kinetics of catalytic conversion of bio-alcohols: theoretical	Matthew John													PhD	M2dcR2	1,2,3,6
Catalytic conversion of bio-alcohols: experimental	Dieter Gunst													PhD	UGent	2,6
Kinetics of catalytic conversion of bio-alcohols: TAP	Rakesh Batchu													PhD	M2dcR2	2,6
Branched higher alcohols from bio-based feedstocks by catalytic processes	Yesid Hernandez													Postdoc	IWT-FISCH	2
Kinetics of biomass pyrolysis & gasification: theoretical	Alper Ince													PhD	ERC-MADP II	1,6
Kinetics of biomass gasification: experimental	Ezgi Toraman													PhD	ERC-MADP II	1,6
Kinetics of biomass pyrolysis model compounds: experimental + modeling	Ruben De Bruycker													PhD	UGent-BOF	1,6
Kinetics of biomass pyrolysis and partial oxidation: experimental + modeling	Shekhar Kulkarni													PhD	IWT-Bioleum	1,6
Chemoinformatics based network generation	Ruben Van De Vijver													PhD	ERC-MADP II	1,6
Renewable feedstocks: sophorolipides	Elisabeth Delbeke													PhD	M2dcR2	1,6
Renewable feedstocks for olefins	Ismaël Amghizar													PhD	Company	1,6
Sustainable production of propylene glycol from glycerine (Bio PG)	Tapas Rajkhowa													PhD	IWT-O&O/i-CaD	2,6
Catalytic Conversion of carbohydrate side streams to develop chemical applications (Carboleum)	Jeroen Poissonnier													PhD	IWT-ICON	2,6
Transformation of bioethanol into hydrocarbons on modified zeolites	Kristof Van der Borgh													PhD	UGent	2,6
Bioethanol selective oxidation into acetaldehyde/acetic acid	Jolien De Waele													PhD	ERC i-CaD	2,6
Stabilization-hydrodeoxygenation of fast pyrolysis oils	Alexandra Bouriakhova													PhD	ERC i-CaD	2,6
XAS-TEM-Modified iron oxide materials for hydrogen production studied by operando XAS and TEM	Aditya Dharanipragada													PhD	FWO	2,3,6
ECO-oil: Enzym- and Cavitation technology for sustainable degumming of vegetable oils	K.Sampaio, J.Tsukamoto													2 Post docs	Company	5,6
Substitution of Latex by biopolymers	L. De Vogelaere													Training	Company	6
Use of microreactor technology for the production of renewable coating intermediates	Marine Movsisyan													junior scientist	Company	5,6
Chemical Modification of insect chitosan	Arno Verlee/Stijn Mincke													PhD	FISCH	6
Biomass fast pyrolysis and gasification -- comprehensive characterization of 'bio-oils'	Li Liu													Postdoc	CSC	1,6
Biomass pyrolysis product separation and characterization	Luc Sy Tran													Postdoc	M2dcR2/IWT	1,6
Cleaning up crude and renewable feeds from nitrogen as a heteroatom	Chetan Raghuveer													PhD	FP7-IWT-Waves	2,6
Conversion of renewable feedstocks to gasoline and base chemicals	Florence Vermeire													PhD	IWT-ARBOREF	6
Elementary reaction networks for the kinetics of the catalytic conversion of renewable resources	Brigitte Devocht													PhD	FWO	1,2,6
Matching cooperative catalysts and operating conditions	Anton De Vylder													PhD	FWO	2
From ab initio to kinetic modelling based catalyst design for deoxygenation	Jenoff De Vrieze													PhD	FWO/ERC i-CaD	2,6
Exploration of continuous flow strategies for the valorisation of renewable resources	Marine Movsisyan													PhD	IWT-Baekeland	4
Alleviating oxidative stress via innovative gold catalysis for an improved biomass production	Arno Verlee													PhD	UGent-BOF	4



Midterm Review by IAB

4. Next steps (1/2)

- relevant focus on
 - design of functional polymers
 - bio-based chemicals and fuels
- attention for further improvement of coherence of the program
 - science:content, methods
 - key messages:insights, applications
 - marketing of results



Midterm Review by IAB

4. Next steps (2/2)

- preparation of succession of program initiator
- adequate measures to be proposed



Management committee (MC)

•Engineering and architecture:

- 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
- Prof. D. Constaes : mathematical analysis
- Prof. D. D'hooge : polymer reaction engineering
- Prof. M. Saeys : kinetics and catalysis
- Prof. M. Sabbe : chemical process technology (01/10/2015)

•Bioscience engineering: Synthesis and Bioresources Chemistry (SynBioC)

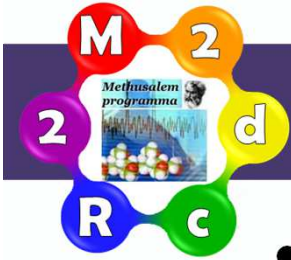
- Prof. C. Stevens : microreactors and renewable feedstocks

•Sciences: Centre for Ordered Materials, Organometalics and Catalysis (COMOC)

- Prof. P. Van der Voort: catalyst synthesis and design

Senior Scientists

Senior Scientists	Research Topic	Subprogram
Hilde Poelman	Physical Characterization Techniques, in particular XAS	P2-P3, P6
Hans-Heinrich Carstensen	Ab initio calculation of rate coefficients of gas phase reactions	P1,P6
Denis Constales	Mathematical analysis of (transient) kinetic data	P5
Grigoriy Yablonsky	Chemical kinetics and chemical engineering	P1
Vladimir Galvita	Catalyst synthesis and testing, CO ₂ capture and utilization	P2-P3,P6



E.Lox 26/07/2013: context

- links with industrial branch roadmaps, H2020, SET plan of EU (comments 6-9)
 - Management committee of 20/11/2013: beyond realm of M2dcR2?
- materials (comment 10)
 - chemical heat pumping
 - combined chemical looping



Coordinator:

Guy B. Marin ('10-'15) Kevin Van Geem ('15-)

Business Development Manager:

Panos Kechagiopoulos ('12-'14)

Stijn Dekeukeleire ('15-)



**UGent's Expertise
for a
Sustainable Chemistry**

Ghent Sustainable Chemistry

- Personnel
 - 27 ZAP
 - 252 researchers
 - 40 technicians
- Current projects: 27.200.000 €
 - Bilateral: 5.900.000 €
 - EU-funding: 14.500.000 €
 - IWT-funding: 6.800.000 €
- Pilot infrastructure: 37.000.000 €



FWO WOG projects

	start	end	M2dcR2 Principal Investigator(s)
Catalysis Research: from Individual Active Sites to Reactors	2015	2019	Martens, Stevens, Marin, Thybaut, Saeys, Reyniers, Van Der Voort
Sustainable Chemistry for the Synthesis of Fine Chemicals	2015	2019	Stevens, Thybaut, Van Geem, Marin

funded PhD's

PhD	research topic	advisors
<u>Steven Pyl</u>	Light olefins from fossil and renewable resources by thermal routes (P1; P6)	GBM, MFR
<u>K. Alexopoulos</u>	Total oxidation of propane by inorganic oxides (P2-P3)	GBM, MFR
<u>Karen Leus</u>	V containing MOF's for selective oxidations (P2-P3)	PVDV, GBM
<u>Carolina Toloza</u>	Kinetic modeling of controlled radical polymerization (CRP) (P4)	MFR, GBM
<u>Ana Cukalovic</u>	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)	CS, GH
<u>Jelena Kovacevic</u>	Process intensification by high-g reactor technology for gas-solid reactions (P5)	GH, GBM

funded PhD's

PhD	research topic	advisors
Marco Djokic	Model steam cracking of gas oils, waxes and vacuum gas oils (P1)	KVG, GBM
Jeroen Lauwaert	Model based design of bifunctional acid/base catalysts for aldol condensations (P2-P3,P6)	JT, PVDV, GBM
Gaoping Xue	Assessment of new FCC technology (MIP) using single-event microkinetics (P1)	JT, GBM, Huixin Weng
<u>Gonzalo Canduela</u>	Multi-scale modeling of benzene hydrogenation on Pd-based bimetallic catalyst (P2-P3)	MFR, GBM
<u>Mike Nguyen</u>	Ab initio study of the zeolite-catalyzed conversion of oxygenates (P2-P3, P6)	MFR, GBM
Elisabeth Delbeke	Innovative sophorolipid and rhamnolipid analogues with tailor-made physico-chemical properties (P6)	CS, KVG
Vinod Kumar	Microkinetic model construction: heterogeneous catalysis (P1-P2)	JT, GBM

funded PhD's

PhD	research topic	Advisors
Yu Zhang	Steam cracking furnace modeling and design (P5)	KVG, GBM, Qian
Isabelle Ascoop	Development of a VO_x/WO_x catalyst on mesoporous titania for the oxidative dehydrogenation of propane (P2)	PV, VG
Mathew John	Conversion of bio-butanol over zeolite catalysts	MFR, GBM
Pieter Verhees	Fouling of convection section of steam cracker	KVG, GH
Stamatis Sarris	Coke formation during steam cracking of heavy hydrocarbon mixtures	KVG, GBM
Aditya Shankar Sandupatla	Atomic layer deposition: a new tool for model based tailoring of acid catalytic activity of microporous, mesoporous and hierarchical materials	MFR, GBM

funded PhD's

PhD	research topic	Advisors
Chetan Raghuveer	Extension of Single Event Micro Kinetic methodology to compounds with hetero atoms and application of gas phase models to liquid phase reactions	JT, GBM
Jiawei Hu	Tri-reforming of biogas by catalyst assisted chemical looping	GBM, VG
Lukas Buelens	Development of materials for CO ₂ capture and conversion	GBM, VG
Natália Olahová	Influence of sulfur compounds on product yields and coke formation during steam cracking of hydrocarbons	KVG, GBM
Nils De Rybel	Kinetic modelling of radical polymerisation, specifically towards RAFT polymerisation	MFR, GBM
Rakesh Batchu	Study the bioethanol transformation into hydrocarbons on modified zeolites catalysts	GBM, VG

funded PhD's

PhD	research topic	Advisors
Rakesh Batchu	Study the bioethanol transformation into hydrocarbon on modified zeolites catalysts	GBM, VG
Jens Dedeyne	Process intensification through reactive flow modulation	KVG,GBM
Yoshi Marien	Modeling of chain length and particle size distribution in radical polymerization	DD, GBM
Lies De Keer	Model-guided design of branched and network polymers	DD, MFR
Alexander Vervust	Multiscale modeling of carbon deposition: from carbon nanotube whiskers to free radical coke formation	KVG,GBM
Brigitte Devocht	Dynamic elementary reaction networks for the kinetics of the catalytic conversion of renewable resources	JT, GBM

funded PhD's

PhD	research topic	Advisors
Anton De Vylder	Exploiting acid base cooperativity and support properties in the synthesis of an innovative aldol condensation catalyst generation	JT, PVDV

Funded Postdoctoral Scientists

Postdoctoral Scientists	Research Topic	Subprogram
Robert Ashcraft	Computational research on rotating powder flow	P5
Maria Pantzali	Computational and Experimental research on powder flow	P5
Tatyana Glazneva	Study of the methane dry reforming mechanism by spectroscopic and transient kinetic experiments	P2-P3
Mike Nguyen	Multi-scale kinetic modeling of controlled radical polymerization processes	P4
<u>Unmesh Menon</u>	Total oxidation of Toluene by Temporal Analysis of Products (TAP)	P2
Amit Mahulkar	CFD of convection section of steam cracker	P5

Funded Postdoctoral Scientists

Postdoctoral Scientists	Research Topic	Subprogram
Evgeniy Redekop	The investigation of a promising catalytic system for propane dehydrogenation, unraveling the mechanism of dehydrogenation and the advancement of scientific toolkit for catalyst characterization	P2
Martin Purino	Ab initio based kinetic modelling of acid catalyzed reactions	P2

Senior Scientists

Senior Scientists	Research Topic	Subprogram
Hilde Poelman	Physical Characterization Techniques, in particular XAS	P2-P3, P6
Hans-Heinrich Carstensen	Ab initio calculation of rate coefficients of gas phase reactions	P1,P6
Denis Constales	Mathematical analysis of (transient) kinetic data	P5
Grigoriy Yablonsky	Chemical kinetics and chemical engineering	P1
Vladimir Galvita	Catalyst synthesis and testing, CO ₂ capture and utilization	P2-P3,P6

Major “spin-off” projects

	start	end	budget /k€	M2dcR2 Principal Investigator(s)
Atomic Layer Deposition (ALD): a new tool for model based tailoring of acid catalytic activity [FWO]	2011	2014	150	Reyniers, Thybaut, Marin
In situ XAS study of ALD of bimetallic materials [FWO]	2011	2014	150	Detavernier, Poelman, Marin
Functional Supramolecular Systems (IUAP VII) [BELSPO]	2012	2017	500	LCT
Multiscale Analysis and Design for Process Intensification and Innovation (MADPII) [FP7-ERC]	2012	2017	2,500	Marin
Model-based Optimization & Control for Process-Intensification and Biopharmaceutical Systems (OPTICO) [FP7-NMP]	2012	2015	290	Reyniers, Marin
Intrinsic Catalytic Kinetics Analyzed and Reconciled with Industrial Conditions (ICKARUS) [FP7-PEOPLE]	2012	2014	170	Redekop, Marin
Ontwikkeling van multi-stap synthesesequenties voor functionele polymeermaterialen door combinatie van één-potprocedures en model gestuurd ontwerp (DOMINO-CLICK) [FWO]	2012	2015	260	Du Prez, Reyniers
Rationeel ontwerp van mesoporeuze koolstof-adsorbentia voor de verwijdering van organische pollutanten uit water [Associatie-UGent]	2012	2016	170	Van Der Voort, Thybaut, Poelman

Major “spin-off” projects

	start	end	budget /k€	M2dcR2 Principal Investigator(s)
Sustainable production of propylene glycol from glycerine (Bio-PG) [IWT, Oleon]	2012	2015	250	D. Packet, Thybaut, Marin
Development of highly selective and stable adsorbents for removal and recycling of rare earths [BOF]	2012	2013	190	Van Der Voort, Thybaut
Catalytic Conversion of carbohydrate side streams to develop new, innovative chemical applications (Carboleum) [IWT-FISCH]	2013	2016	240	Thybaut, Marin
Ab initio based multiscale modeling of controlled radical polymerization [FWO]	2013	2016	280	Reyniers, Heynderickx
Modified iron oxide materials for hydrogen production studied by operando XAS and TEM [FWO]	2013	2016	280	G. Van Tendeloo, Poelman, Marin
Periodic Mesoporous Organosilica (PMO) as bifunctional acid/base catalysts [FWO]	2013	2016	180	Van Der Voort, P. Cool, Thybaut
FAST industrialization by CAtalysts R&D (FASTCARD) [FP7-NMP]	2014	2017	800	Thybaut, Galvita, Reyniers, Marin
Innovative Catalyst Design for Large-Scale, Sustainable Processes (i-CaD) [FP7-ERC]	2014	2019	2 000	Thybaut

Major “spin-off” projects

	start	end	budget /k€	M2dcR2 Principal Investigator(s)
Bioleum Fuels and Chemicals by fast pyrolysis of biomass [IWT-SBO]	2014	2018	745	Van Geem, Marin
COILSIM - An advanced simulation and optimization software for the ethylene industry [IOF-Advanced]	2014	2015	150	Van Geem, Marin
Confidential	2014	2019	confidential	Van Geem, Heynderickx, Reyniers, Marin
Modelling-guided Design of Selective Catalytic Processes [FWO-Odyseus]	2014	2019	2 475	Saeys
Improving Cracking Furnace Availability by Evaluating Anti-coking Technologies, Improved Operational Protocols and Modeling and by Investigating Coke-metal Furnace Interactions (ICrA) [TOTAL]	2014	2018	450	Van Geem, Marin
Olefin Production from Fossil and Renewable Feedstocks [SABIC]	2014	2018	300	Van Geem, Marin
COILSIM – An Advanced Simulation and Optimization Software for the Ethylene Industry	2014	2015	150	Van Geem, Marin

Major “spin-off” projects

	start	end	budget /k€	M2dcR2 Principal Investigator(s)
Alleviating Oxidative Stress via Innovative Gold Catalysis for an Improved Biomass Production [BOF-IOP]	2014	2018	400	Van Breusegem, Stevens
Development of a Center of Expertise and Pilot Production Installation for Industrial Flow Processes in Flanders [IWT-FISCH-ICON]	2014	2016	4 550 (total)	Stevens

Individual fellowships

	Start	end
Maarten Sabbe: First-principles design of transition metal hydrocarbon hydrogenation catalysts: beyond model catalysts [FWO-postdoc]	2009	2015
Carl Schietekat: Computational fluid dynamics based design of steam cracking reactors using detailed kinetic models [FWO]	2011	2015
Dagmar D'hooge: Development of a multi-scale modeling platform for optimization of radical polymerization processes [FWO-postdoc]	2012	2015
Pieter Derboven: Multi-scale modeling of reversible addition-fragmentation chain transfer polymerization [IWT]	2012	2015
Nick Vandewiele: Development of Automatic Reaction Network Generation Technology: 3D Structure & Reactivity Implementation [FWO]	2012	2014
Jonas Van Belleghem: Multi scale modelling of complex kinetics on metal catalysts: Fischer Tropsch synthesis [FWO]	2012	2016
Yu Zhang: Large eddy simulation of steam cracking furnaces [CSC]	2012	2014
Mieke Meire: Mesoporeuze titania structuren met geïncorporeerde edelmetaal nanodeeltje: Een uiterst actieve fotokatalysator	2012	2016

Individual fellowships

	Start	end
David Van Cauwenberge: Simulation and design of novel steam cracking reactors and furnaces using Computational Fluid Dynamics [IWT-Baekeland]	2013	2017
Ruben Van de Vijver: Automated reaction network generation of hetero-atomic mixtures using 3D representations of molecules [IWT]	2014	2016
Pieter Reyniers: First-principles 3D reactor design: large eddy simulation and direct numerical simulation with detailed chemistry [FWO/BOF]	2014	2016
Marine Movsisyan: Exploration of continuous flow strategies for the valorization of renewable resources [IWT-Baekeland]	2014	2016
Melissa Van Overtveldt: Synthesis of strigolactone and karrikin analogues by gold mediated cyclization [FWO]	2014	2016
Yoran De Vos: Attritie-resistente zuurstofdragers voor chemical looping reforming door optimalisatie van de microstructuur [VITO]	2014	2018
Guangbo Wang: Functional metal-organic frameworks: tuning of flexible frameworks for efficient gas separation [CSC/BOF]	2014	2016
Jiawei Hu: Computational fluid dynamics study of steam cracking furnaces	2014	2016

Individual fellowships

	Start	end
Songjun Liu: Reaction kinetics and reactor design fro the short contact time partial oxidation of methane [CSC/FP7]	2014	2016
Lukas Buelens: Development of Novel Materials for Carbon dioxide Capture and Conversion (DyNaMiC ³) [IWT]	2015	2018

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: M.-F. Reyniers and G. B. Marin

May, 2010

Defended Ph D theses in 2011

- Modeling of Reaction, Attrition and Breakage in Gas-Solid Multiphase Flow Systems Using the Quadrature Method Approach

Abhishek Dutta

Advisors: Heynderickx, G.J.; Constaes, D.

January 2011

- Mathematical determination of reaction networks from transient kinetic experiments

Raf Roelant

Advisors: Constaes, 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 Ph D theses in 2011

➤ Ab Initio Study of the Adsorption of Hydrocarbons in Zeolites: Influence of Molecular Structure and Framework Topology

Bart De Moor

Advisors: Marin, G.B.; Reyniers, M.-F.

February 2011

Defended Ph D 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: Thybaut, J.W.; Marin, G.B.

March 2012

- Design and Experimental Study with Laser Doppler Anemometry of a Circulating Fluidized Bed

Gorik Van engelandt

Advisors: Heynderickx, G.J.; Marin, G.B.

July 2012

- Hydrocarbon Oxidation over Metal Oxide Catalysts: an Ab Initio and Operando X-Ray Absorption Study

Konstantinos Alexopoulos

Advisors: Marin, G.B.; Reyniers, M.-F.

August 2012

Defended Ph D theses in 2012

- Sustainable Production of Light Olefins: from Fossil to Renewable Resources

Steven Pyl

Advisors: Reyniers, M.-F.; Marin, G.B.

October 2012

- Use of microreactor technology and renewable resources to develop green chemical processes

Ana Cukalovic

Advisors: Stevens, C.V.; Heynderickx, G.J.

December 2012

- Stochastic Modeling of Radical Polymerizations

Paul H.M. Van Steenberge

Advisors: Marin, G.B.; Reyniers, M.-F.

December 2012

- The development of vanadium and titanium containing metal organic frameworks for applications in adsorption and heterogeneous catalysis

Karen Leus

Advisors: Van Der Voort, P.; Marin, G.B.

December 2012

Defended Ph D theses in 2012

- Micokinetics of the Liquid-Phase alkylation of benzene with octenes over Y zeolites:
effect of acidity

Iftemie Ionel Craciun

Advisors: Marin, G.B.; Reyniers, M.-F.

December 2012

Defended Ph D theses in 2013

- Toluene Total Oxidation over CuO-CeO₂/Al₂O₃: Structural and Kinetic Characterization

Unmesh Menon

Advisors: Marin, G.B.; Galvita, V.V.

January 2013

- Model Based Design of Functional Polymer Materials by Initiators for Continuous Activator Regeneration Atom Transfer Radical Polymerization (ICAR ATRP)

Carolina de los Angeles Toloza Porras

Advisors: Reyniers, M.-F.; Marin, G.B.

February 2013

- Quantitative Understanding of Zeolite Catalyzed Conversion of Oxygenates to Liquids by Single-Event Microkinetics

Pravesh Kumar

Advisors: Thybaut, J.W.; Marin, G.B.

February 2013

- First Principles Microkinetic Modelling of Bio-Alcohols Dehydration: Influence of Zeolite Acidity and Topology

Cuong Manh Nguyen

Advisors: Reyniers, M.-F.; Marin, G.B.

March 2013

Defended Ph D theses in 2014

- Kinetic Study of the (Trans)Esterification Catalyzed by Gel and Macroporous Resins

Evelien Van de Steene

Advisors; Thybaut J.W.; De Clercq J.

April 2014

- Kinetic Model Construction Using Chemoinformatics

Nick Vandewiele

Advisors: Reyniers, M.-F.; Marin, G.B.

May 2014

- Mastering Diffusion, Confinement and Acid Strength in Zeolites for the Alternative Production of Conventional Fuels and Chemicals

Bart Vandegehuchte

Advisors: Thybaut, J.W.; Marin, G.B.

June 2014

- Steam Cracking: from Feedstock Analysis to Plant Optimization

Thomas Dijkmans

Advisors: Van Geem, K.M.; Marin, G.B.

September 2014

Defended Ph D theses in 2014

- Influence of the Reactor Coil Material on Coke Formation during Steam Cracking of Hydrocarbons

Andres Muñoz Gandarillas

Advisors: Reyniers, M.-F.; Marin, G.B.

October 2014

- An Intrinsic Kinetics Based Methodology for Multi-Scale Modeling of Chemical Reactions

Kenneth Toch

Advisors: Thybaut, J.W.; Marin, G.B.

December 2014

- Cold Flow Study of a Gas-Solid Vortex Reactor

Jelena Kovacevic

Advisors: Heynderickx, G.J.; Marin, G.B.

December 2014

Defended Ph D theses in 2015

- First Principles Based Design of Bimetallic Catalysts for Benzene Hydrogenation

Gonzalo Canduela Rodriguez

Advisors: Reyniers, M.-F.; Sabbe, M.K.

February 2015

- Computational fluid dynamics based design of steam cracking reactors using detailed kinetic models

Carl Schietekat

Advisors: Marin, G.B.; Van Geem, K.

June 2015

- Design of Cooperative Acid-Base Catalysts for Aldol Condensations

Jeroen Lauwaert

Advisors: Thybaut, J.W.; Marin, G.B.

September 2015

- Alternative Design of Pt-Based Catalysts: an X-Ray Spectroscopic View

Matthias Filez

Advisors: Marin, G.B.; Detavernier, C.

October 2015

Defended Ph D theses in 2015

- Sustainable conversion of biomass oxygenates: ab initio based model simulation

Paschalis Paraskevas

Advisors: Marin G.B.; Reyniers M.-F.

October 2015

- Pyrolysis kinetics of fossil and renewable fuels

Marko Djokic

Advisors: Van Geem K.; Marin G.B.

November 2015

Publications

2009

Probability Density Function simulation of Turbulent Reactive Gas-Solid Flow in a Riser, *S.N.P. Vegendla, G.J. Heynderickx, G.B. Marin*

Chemical Engineering and Technology, 32, 3, 492–500, 2009, SCI-IF: 0.923 (2008)

Modeling the evaporation of a hydrocarbon feedstock in the convection section of a steam cracker, *S.C.K. De Schepper, G.J. Heynderickx, G.B. Marin*

Computers and Chemical Engineering, 33, 122-132, 2009, SCI-IF: 1.755 (2008)

Physisorption and chemisorption of alkanes and alkenes in H-FAU: a combined ab initio – statistical thermodynamics study, *B.A. De Moor, M.-F. Reyniers, G.B. Marin*

Physical Chemistry Chemical Physics, 11, 2939-2958, 2009, SCI-IF: 4.064 (2008)

Importance of radical transfer in precipitation polymerization: the case of vinyl chloride suspension polymerization, *J. Wieme, D.R. D'hooge, M.-F. Reyniers, G.B. Marin*

Macromolecular Reaction Engineering, 3(1), 16-35, 2009., SCI-IF: 1.041 (2008)

Methodology for kinetic modeling of atom transfer radical polymerization

D.R. D'hooge, M.-F. Reyniers, G.B. Marin

Macromolecular Reaction Engineering, 3 (4), 185-209, 2009, SCI-IF: 1.041 (2008)

Publications

2009

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 (8), 2159-2170, 2009, SCI-IF: 1.883 (2008)

Microkinetic modelling of structural properties of poly(vinyl chloride)
J. Wieme, M.-F. Reyniers, G.B. Marin, **Macromolecules**, 42 (20), 7797-7810, 2009, SCI-IF: 4.407 (2008)

Synergy between shape selective and non shape selective bifunctional zeolites modeled via the Single-Event MicroKinetic (SEMK) methodology
I.R. Choudhury, J.W. Thybaut, P. Balasubramanian, J.F.M. Denayer, J.A. Martens, G.B. Marin, **Chemical Engineering Science**, 65, 174-178, 2009, SCI-IF: 1.884 (2008)

Coke formation in the Transfer Line Exchanger (TLE) during steam cracking of hydrocarbons, *K.M. Van Geem, I. Dhuyvetter, S. Prokopiev, M.-F. Reyniers, D. Viennet, G.B. Marin*, **Industrial and Engineering Chemistry Research**, 48 (23) 10343-10358, 2009, SCI-IF: 1.895 (2007)

Publications

2009

A new approach to diagnostics of ideal and non-ideal flow patterns: The concept of reactive-mixing index (REMI) analysis, *Yablonsky, G.S., Constales, D., Marin, G.B.*, **Chemical Engineering Science**, 64, 4875 – 4883, 2009, SCI-IF: 1.884 (2008)

Coupled simulation of the flue gas and process gas side of a steam cracker convection section, *De Schepper, S.C.K., Heynderickx, G.J., Marin, G.B.*, **AIChE Journal**, 55, 2773-2787, 2009, SCI-IF: 2.370 (2008)

Kinetic modeling of the total oxidation of propane over anatase and vanadia sputter deposited catalysts, *Heynderickx, P.M., Thybaut, J.W., Poelman, H., Poelman, D., Marin, G.B.*, **Applied Catalysis B: Environmental**, 92, 295-306, SCI-IF: 4.853 (2008)

Temporal analysis of products reactor as a complementary tool to study the mechanism of some green catalytic reactions, *Olea, M., Tada, M., Iwasawa, Y., Balcaen, V., Sack, I., Poelman, D., Marin, G.B., Poelman, H.*, **J. Chemical Engineering of Japan**, 42, s219-s225, 2009, SCI-IF: 0.569 (2008)

Deposition and characterization of vanadium oxide thin films: linking single crystal and supported catalyst, *Poelman, H., Silversmit, G., Poelman, D., Marin, G.B., Sels, B.S.*, **Catalysis Today**, 142, 125-131, 2009, SCI-IF: 3.004 (2008)

Publications

2009

In-situ XAS study on the Cu and Ce local structural changes in a CuO-CeO₂/Al₂O₃ catalyst under propane reduction and re-oxidation, *Silversmit, G., Poelman, H., Balcaen, V., Heynderickx, P.M., Olea, M., Nikitenko, S., Bras, W., Smet, P.F., Poelman, D., De Gryse, R., Reyniers, M.-F., Marin, G.B.*, **J. Phys. Chem. Solids**, 70 1274-1284 2009, SCI-IF: 1.103 (2008)

Design of Optimum Zeolite Pore System for Central Hydrocracking of Long-chain n-Alkanes based on a Single-Event MicroKinetic Model, *Thybaut, J.W., Choudhury, I.R., Denayer, J.F., Baron, G.V., Jacobs, P.A., Martens, J.A., Marin, G.B.*, **Topics in Catalysis**, 52 (9), 1251-1260, 2009, SCI-IF: 2.212 (2008)

Publications

2010

Rotating Fluidized Bed with a Static Geometry: Guidelines for design and operating conditions, *A. Dutta, R.P. Ekatpure, G.J. Heynderickx, A. de Broqueville, G.B. Marin* **Chemical Engineering Science**, 65, 1678–1693, 2010, SCI-IF: 2.136 (2009)

Hydrogen radical addition to unsaturated hydrocarbons and reverse beta-scission modeling of activation energies and pre-exponential factors, *M.K. Sabbe, M.-F. Reyniers, M. Waroquier, G.B. Marin*, **ChemPhysChem**, 11, 1, 195-210, 2010, SCI-IF: 3.453 (2009)

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Modeling the influence of resonance stabilization on the kinetics of hydrogen abstractions , *M.K. Sabbe, A.G. Vandeputte, M.-F. Reyniers, M. Waroquier, G.B. Marin* **Physical Chemistry Chemical Physics**, 12, 6, 1278-1298, 2010, SCI-IF: 4.116 (2009)

Publications

2010

A Microkinetic Vision on High-Throughput Catalyst Formulation and Optimization: Development of an Appropriate Software Tool, *K. Metaxas, J.W. Thybaut, G. Morra, D. Farrusseng, C. Mirodatos, G.B. Marin*, **Topics in Catalysis**, 53, 64-76, 2010, SCI-IF: 2.379 (2009)

Initiator efficiency modeling for vinyl chloride suspension polymerization
J. Wieme, M.-F. Reyniers, G.B. Marin, **Chemical Engineering Journal**, 154, 203-210, 2010, SCI-IF: 2.816 (2009)

Steady-state simulation of Fluid Catalytic Cracking riser reactors using a decoupled solution method with feedback of the cracking reactions on the flow
E. Baudrez, G.J. Heynderickx, G.B. Marin, **Chemical Engineering Research and Design**, 88, 290-303, 2010, SCI-IF: 1.223 (2009)

Simulation of an industrial riser for catalytic cracking in the presence of coking using Single-Event MicroKinetics, *R. Quintana-Solorzano, J.W. Thybaut, P. Galtier, G.B. Marin*, **Catalysis Today**, 150, 319-331, 2010, SCI-IF: 3.526 (2009)

Publications

2010

Identifiability of Rate Coefficients in Linear Reaction Networks from Isothermal Transient-Experimental Data, *Roelant, R., Constales, D., Van Keer, R., Marin, G.B.*, **Chemical Engineering Science**, 65, 2333–2343, 2010, SCI-IF: 2.136 (2009)

Modeling the coke formation in the convection section tubes of a steam cracker
S.C.K. De Schepper, G.J. Heynderickx, G.B. Marin
Industrial & Engineering Chemistry Research, 49, 12, 5752–5764, 2010, SCI-IF: 1.758 (2009)

Micromixing effects on Series-Parallel and Autocatalytic Reactions in a Turbulent Single-Phase Gas Flow, *S.N.P. Vegendla, G.J. Heynderickx, G.B. Marin*
Chemical Engineering Science, 65, 4621–4629, 2010, SCI-IF: 2.136 (2009)

Theoretical study of the adsorption of C1-C4 primary alcohols in H-ZSM-5
C.M. Nguyen, M.-F. Reyniers, G.B. Marin, **Physical Chemistry Chemical Physics**, 12, 9481-9493, 2010, SCI-IF: 4.116 (2009)

Publications

2010

Atom Transfer Radical Polymerization of Isobornyl Acrylate: a Kinetic Modeling Study
D.R. D'hooge, M.-F. Reyniers, F.J. Stadler, B. Dervaux, C. Bailly, F.E. Du Prez, G.B. Marin, **Macromolecules**, 43, 8766-8781, 2010, SCI-IF: 4.539 (2009)

Theoretical study of the thermal decomposition of dimethyl disulfide, *A.G. Vandeputte, M.-F. Reyniers, G.B. Marin*, **Journal of Physical Chemistry A**, 114, 39, 10531–10549, 2010, SCI-IF: 2.899 (2009)

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*
AIChE Journal, 56, 12, 3174-3188, 2010, SCI-IF: 1.955 (2009)

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*, **Journal of Chromatography A**, 1217, 43, 6623-6633, 2010, SCI-IF: 4.101 (2009)

Accurate High-Temperature Reaction Networks for Alternative Fuels: Butanol Isomers
K.M. Van Geem, M.R. Harper, S.P. Pyl, G.B. Marin, W.H. Green
Industrial & Engineering Chemistry Research, 49, 21, 10399-10420, 2010, SCI-IF: 1.758 (2009)

Publications

2010

The remarkable catalytic activity of the Saturated Metal Organic Framework V-MIL-47 in the cyclohexene oxidation, *K. Leus, I. Muylaert, M. Vandichel, G.B. Marin, M. Waroquier, V. Van Speybroeck, P. Van Der Voort*, **Chemical Communications**, 46, 5085-5087, 2010, SCI-IF: 5.500 (2009)

A coordinative saturated vanadium containing metal organic framework that shows a remarkable catalytic activity, *K. Leus, I. Muylaert, V. Van Speybroeck, G.B. Marin, P. Van Der Voort*, **Studies in Surface Science and Catalysis**, 175, 329-332, 2010, (WOS proceeding paper)

Kinetics of Substituted Silylene Addition and Elimination in Silicon Nanocluster Growth Captured by Group Additivity, *Adamczyk, A.; Reyniers, M.-F.; Marin, G.B.; Broadbelt, L.*, **Chemphyschem**, 11(9) 1978-1994, 2010, SCI-IF: 3.339 (2010)

Kinetic correlations for H-2 addition and elimination reaction mechanisms during silicon hydride pyrolysis, *Adamczyk, A.; Reyniers, M.-F.; Marin, G.B.; Broadbelt, L.*, **Physical Chemistry Chemical Physics**, 12(39) 12676-12696, 2010, SCI-IF: 4.116 (2009)

Theoretical study of the effect of (001) TiO₂ anatase support on V₂O₅, *Alexopoulos, K., Hejduk, P., Witko, M., Reyniers, M.-F., Marin, G.B.*, **Journal of Physical Chemistry C**, 114 (7) 3115-3130, 2010, SCI-IF: 2.899 (2009)

Publications

2010

Time-resolved operando X-ray absorption study of CuOCeO₂/Al₂O₃ catalyst during total oxidation of propane, *Alexopoulos, K., Anilkumar, M., Reyniers, M.-F., Poelman, H., Cristol, S., Balcaen, V., Heynderickx, P.M., Poelman, D., Marin, G.B.*, **Appl. Catal. B**, 97, 381-388, 2010, SCI-IF: 5.252 (2009)

TAP study on the active oxygen species in the total oxidation of propane over a CuO-CeO₂/g-Al₂O₃ catalyst, *Balcaen, V., Roelant, R., Poelman, H., Poelman, D., Marin, G.B.*, **Catalysis Today**, 157, 49-54, 2010, SCI-IF: 3.526 (2009)

Mathematics in chemical kinetics and engineering : Preface to the MaCKiE-2009 special issue, *Constales, D., Van Keer, R., Marin, G.B., Heynderickx, G.J.*, **Chemical Engineering Science**, 65, 2265-2266, 2010, SCI-IF: 2.136 (2009)

Coincidences in chemical kinetics: Surprising news about simple reactions, *Yablonsky, G.S.; Constales, D.; Marin, G.B.*, **Chemical Engineering Science**, 65, 23, 6065-6076, 2010, SCI-IF: 2.136 (2009)

A new Ultra Stable Mesoporous Adsorbent for the Removal of Mercury, *De Canck E., Lapeire L., De Clerq J., Verpoort F. and Van Der Voort P.*, **Langmuir**, 26(12), 10076-10083, 2010

Publications

2010

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Catalyst-assisted chemical looping for CO₂ conversion to CO, *Galvita, V.V.; Poelman, H.; Detavernier, C.; Marin, G.B.*, **Applied Catalysis B: Environmental**, 164, 184–191, 2015, SCI-IF: 6.002 (2013)

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2015

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Experimental and computational study of the initial decomposition of gamma-valerolactone, *De Bruycker, R.; Carstensen, H.-H.; Simmie, J.; Van Geem, K.M.; Marin, G.B.*, **Proceedings of the Combustion Institute**, 35, 515-523, 2015, SCI-IF: 3.828 (2013)

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Exploring the Full Potential of Reversible Deactivation Radical Polymerization Using Pareto-Optimal Fronts, *Fierens, S.; D'hooze, D.R.; Van Steenberge, P.; Reyniers, M.-F.; Marin, G.B.*, **Polymers**, 7 (4), 655-679, 2015, SCI-IF: 2.505 (2013)

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Spacing and Acid Strength Effects on Acid-Base Cooperatively-Catalyzed Aldol Condensation on Aminosilica Materials, *Lauwaert J., Moschetta E.G., Van Der Voort P., Thybaut J.W., Jones C.W., Marin G.B.*, **Journal of Catalysis**, 325, 19-25, 2015, SCI-IF: 6.073 (2013)

Three-component particle velocity measurements in the bottom section of a riser , *Pantzali, M.N.; De Ceuster, B.; Marin, G.B.; Heynderickx, G.J.*, **International Journal of Multiphase Flow**, 72, 145-154, 2015, SCI-IF: 1.943 (2013)

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Tuning the Pore Geometry of Ordered Mesoporous Carbons for Enhanced Adsorption of Bisphenol-A, *Libbrecht W., Vandaele K., De Buysser K., Verberckmoes A., Thybaut J.W., Poelman H., De Clercq J., Van Der Voort P.*, **Materials**, 8, 1652-1665, 2015, SCI-IF: 1.879 (2013)

Predicting kinetic dependences and closing the balance: Wei and Prater revisited, *Constales, D.; Yablonsky, G.S.; Marin, G.B.*, **Chemical Engineering Science**, 123, 328-333, 2015, SCI-IF: 2.613 (2013)

When the Final Catalyst Activity Profile Depends Only on the Total Amount of Admitted Substance: Theoretical Proof, *Constales, D.; Yablonsky, G.S.; Phanawadee, P.; Pongboutr, N.; Limtrakul, J.; Marin G.B.*, **AIChE Journal**, 61 (1), 31-34, 2015, SCI-IF: 2.581 (2013)

A new class of antimicrobial biosurfactants: quarternary ammonium sophorolipids, *Delbeke, E.I.P., Roman B.I., Marin G.B., Van Geem K.M., Stevens C.V.*, **Green Chemistry**, published on line, 2015, SCI-IF: 6.852 (2013)

Singlet-oxygen oxidation of 5-hydroxymethylfurfural in continuous flow, *Heugebaert, T.S.; Stevens C.V.; Kappe, C.O.*, **ChemSusChem** 8 (10), 2015, SCI-IF: 7.117 (2013)

TOP-10 Publications

On-line analysis of complex hydrocarbon mixtures using comprehensive two-dimensional gas chromatography, *Van Geem, K.M., Pyl, S.P., Reyniers, M.-F., Vercammen, J., Beens, J., Marin, G.B.*, **Journal of Chromatography A**, 1217 (43), 6623-6633, 2010, SCI-IF: 4.101 (2009)

Adsorption of C2-C8 n-alkanes in zeolites, *De Moor, B.A., Reyniers M.-F., Gobin O.C., Lercher, J.A., Marin, G.B.*, **Journal of Physical Chemistry C**, 115, 1204-1219, 2011, SCI-IF: 4.520 (2010)

Comprehensive reaction mechanism for n-butanol pyrolysis and combustion, *Harper, M.R., Van Geem, K.M., Pyl, S.P., Marin, G.B., Green, W.H.*, **Combustion and Flame**, 158 (1), 16-41, 2011, SCI-IF: 2.747 (2011)

Origin of the difference in branching in acrylate polymerization under controlled and free radical conditions: a computational study, *Konkolewicz, D., Sonoswski, K., D'hooge, D.R., Szymanski, R., Reyniers, M.-F. Marin, G.B., Matyjaszewski, K.*, **Macromolecules**, 44, 8361, 2011, SCI-IF: 4.539 (2009)

First principle-based simulation of ethane steam cracking, *Sabbe, M.K., Van Geem, K.M., Reyniers, M.-F., Marin, G.B.*, **AIChE Journal**, 57 (2), 482-496, 2011, SCI-IF: 2.030 (2010)

Kinetics of Chemical Reactions : Decoding Complexity, *Marin, G.B., Yablonsky, G.S.*, **Wiley-VCH Verlag**, 446 pages, 2011, ISBN 978-3-527-31763-9, 2011

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Modeling Fast Biomass Pyrolysis in a Gas-Solid Vortex Reactor, *Ashcraft, R.W., Heynderickx, G.J., Marin, G.B.*, **Chemical Engineering Journal**, 207-208, 195-208, 2012, SCI-IF: 3.461 (2011)

Nature of the active sites in the total oxidation of toluene over CuO-CeO₂/Al₂O₃, *Menon U., V. Galvita, H. Poelman, G.B. Marin*, **Journal of Catalysis**, 295, 91-103, 2012, SCI-IF: 6.002 (2011)

Experimental and Theoretical Methods in Kinetic Studies of Heterogeneously Catalyzed Reactions, *Reyniers M.-F., Marin G.B.*, **Annual Review of Chemical and Biomolecular Engineering**, 5, 563-594, 2014, SCI-IF: 8.109 (2013)

Spacing and Acid Strength Effects on Acid-Base Cooperatively-Catalyzed Aldol Condensation on Aminosilica Materials, *Lauwaert J., Moschetta E.G., Van Der Voort P., Thybaut J.W., Jones C.W., Marin G.B.*, **Journal of Catalysis**, 325, 19-25, 2015, SCI-IF: 6.073 (2013)

M2dcR2 $\Rightarrow$ Applications – FP7/H2020

- *H2020-ERC-StG-2015: In-silico deSign Of Functional Advanced Macromolecules (ISOFAM) [February 2015]*

D. D'hooge

- *H2020-ERC-CoG-2015: High Performance Reactor and Reaction Engineering (HYPER²) [April 2015]*

K. Van Geem

- *H2020-SC5-2015-two-stage: New Model Based Tools for Improvement of Catalytic Exhaust Gas Cleaning Systems (IMPACT) [April 2015]*

V. Galvita, J.W. Thybaut, G.B. Marin

M2dcR2 $\Rightarrow$ Applications - FWO

- **FWO: Model-based Optimization of Nanostructured Bimetallic Pt-catalysts for (de)Hydrogenation Reactions [March 2015]**
M.-F. Reyniers, C. Detavernier, H. Poelman
- **FWO: Combining Molecular Modeling, Intrinsic Kinetics, and In Situ Characterization to Unravel the Role of Boron, a Versatile Promoter in Catalysis (ComBo) [March 2015]**
M. Saeys, K. Foettinger
- **FWO: Experimental and Numerical Study of Dilute Gas-Solid Riser Flow [March 2015]**
G. Heynderickx
- **FWO: Selective Catalytic Dehydrogenation of Light Alkanes: Materials, Kinetics and Reactor [April 2015]**
V. Galvita, M. Saeys, J. Levec
- **FWO: Process Intensification via Non-thermal Plasma Catalysis [April 2015]**
G. Stefanidis, K. Van Geem

M2dcR2 $\Rightarrow$ Applications - BOF

- GOA: Prediction of Turbulent Reactive Flows by means of Numerical Simulation (PRETREF) [April 2015]

B. Merci, I. Nopens, K. Van Geem, S. Verhelst, S. Verstockt, J. Vierendeels

M2dcR2 $\Rightarrow$ Applications - Francqui

➤ *FRANCQUI (International Francqui Professor): Rodney Fox [May 2015]*

K. Van Geem, G.B. Marin

M2dcR2⇒Applications - individual fellowships

- Dagmar D'hooge: Model-based design of macromolecular architectures for functional polymeric applications [FWO-postdoc-2nd term]
- Paul Van Steenberge: Stochastic modeling of radical polymerizations [FWO-postdoc-1st term]
- Brigitte Devocht: Dynamic elementary reaction networks for the kinetics of the catalytic conversion of renewable resources [FWO]
- Alexander Vervust: Multiscale modeling of carbon deposition: from carbon nanotube whiskers to free radical coke formation [FWO]
- Judith Ouwehand: Development of chiral acid-base heterogeneous catalysts by functionalization of PMO materials through click-chemistry reactions [BOF]

M2dcR2 $\Rightarrow$ Applications in 2011 -not honoured- FP7

- **FP7-PEOPLE-2010-ITN: Highly Selective Catalysts for Alkene Oxidation through Fundamental Understanding (4selox)**
P. Ellis, Y. Schuurman, G. Hutchings, G.B. Marin, M.-F. Reyniers, J. Thybaut, J.-D. Grunwaldt, I. Hermans, G. Jones
- **FP7-ENERGY-2011-1: Development of a fully integrated process for the decentralized production of stabilised pyrolysis oil from sustainable biomass (PICULA)**
J. Winkelman, E. Heeres, R. Venderbosch, Dr. Y. Solantausta, R. Diaz-Chavez, W. Prins, G.B. Marin, K. Van Geem, V. Yakovlev, F. Vogel, K. Warsicki, A. Sirven, N. Szarka, S. Pütz, J. Boucher
- **FP7-ENERGY-2012-1-2STAGE : Solutions for Utilizing CarboHydrates As Renewable Alternatives (SUCHARA)**
H.J. Heeres, R. Venderbosch, P.J. Schoenmaker, R. Parton, K. Van Geem, G.B. Marin, W. Leitner, A. Corma, V. Yakovlev, D. Meier, P. Westermann, B. Zwiijnenburg, M. Watson
- **ERC-2011-StG (Starter Grant): Model Guided Design of the Catalytic Transformation of Biomass into Fuels and Chemicals (CatBiChem)**
J. Thybaut

M2dcR2 $\Rightarrow$ Applications in 2011 -not honoured- FP7

- *FP7-PEOPLE-2011-ITN: Advanced training in knowledge oriented High throughput CATalysis for the bio-based economy (HICAT)*

M.-F. Reyniers, J. Thybaut, G.B. Marin

M2dcR2 $\Rightarrow$ Applications in 2010 -not honoured- IWT

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

C. Stevens, T. Van Gerven, J. Denayer, L. Diels, G. Heynderickx, J. Van Impe, J. Dewulf, J. Lammertyn, K. Van Aken

- **SBO: Rational Design of Industrial Catalysts (INCA)**

J. Paul, G. Huyberechts, P. Van Der Voort, J. Thybaut, A. Verberckmoes, J. De Clercq, B. Sels

M2dcR2 $\Rightarrow$ Applications in 2011-not honoured -FWO

- *FWO*: Experimental and computational study of micro reactor technology for reactions with diazomethane (MICROREACTOREN)

G. Heynderickx, C. Stevens

- *FWO*: Experimental and computational analysis of particle behavior in the FCC process (FCC-process)

G. Heynderickx, I. Nopens

- *FWO*: 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

M2dcR2 $\Rightarrow$ Applications in 2010 -not honoured- MRP

- *MRP (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

M2dcR2 $\Rightarrow$ Applications in 2011 -not honoured- BOF

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

M.-F. Reyniers, K. Van Geem, W. Prins, W. Boerjan, B. Vanholme, J. Martins, F. Ronsse

M2dcR2 $\Rightarrow$ Applications in 2012 -not honoured- FP7

- **FP7-NMP-2012-SMALL-6: Ultra Performance Low Impact Fischer-Tropsch (UPLIFT)**

D. Farrusseng, Y. Schuurman, J.L. Rousset, C. Mirodatos, C. Thieuleux, A. Quadrelli, E. Tsang, E. Shotton, A. Kroner, G.B. Marin, M.-F. Reyniers, G. Kelly, S. Ellis, D. James, P. Ellis

- **FP7-NMP-2012-SMALL-6: Catalysis In Renewable Oil Production (CIROP)**

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

- **FP7-PEOPLE-2011-ITN: Highly Selective Catalysts for Alkene Oxidation through Fundamental Understanding (4selox) [aanvraag jan. 2012]**

P. Ellis, Y. Schuurman, G. Hutchings, G.B. Marin, M.-F. Reyniers, J. Thybaut, J.-D. Grunwaldt, I. Hermans, G. Jones

M2dcR2 $\Rightarrow$ Applications in 2012 -not honoured- FP7

- *FP7-PEOPLE-2012-IAPP: Lignocellulosic Biomass Conversion for the Production of Light Olefins (Biolefins)*

G.B. Marin, M. Ruitenbeek, F. Van Damme

- *FP7-NMP-2013-two-stage: Seamless from nano to the reactor: multiscale numerical framework for catalytic reaction modeling and design (Multi-CReaM)*

G.B. Marin, M.-F. Reyniers, J. Thybaut

- *FP7-PEOPLE-2012-CIG: Theoretical and Experimental Characterization of the Pyrolysis Chemistry of Phenols and Phenyl Ethers (TEChP3)*

H.H. Carstensen

- *ERC-2013-StG: Biomass Reaction Engineering Driving Genetic Modification (BRiDGe)*

K. Van Geem

M2dcR2 $\Rightarrow$ Applications in 2012 -not honoured- FWO

- *FWO*: Joint kinetics of reciprocal experiments (JoKiREx)

G.B. Marin, D. Constaes

- *FWO*: Pyrolysis of organic waste streams, activation and regeneration of activated carbon using microwave heating (Micro-Pyro)

J. Yperman, R. Carleer, K. Van Geem

- *FWO*: First principles based multi-scale modeling of controlled radical polymerisation processes (MULTISCALECRP)

M.-F. Reyniers, G. Heynderickx

M2dcR2 $\Rightarrow$ Applications in 2012 -not honoured- BOF

➤ **BOF-GOA: Solar Hydrogen: fueling the future (SoHy)**

D. Poelman, I. Van Driessche, J. Thybaut, A. Adriaens, H. Poelman,
K. De Buysser, P. Lommens

➤ **BOF-GOA: Compositional Analysis of Lignocellulosic Bio (ALiBi)**

M.-F. Reyniers, W. Boerjan, J.C., J.C. Martins, K. Van Geem, F.
Lynen, K. Morreel

➤ **BOF-GOA: Computational study of particle attrition, breakage and aggregation in gas-solid two-phase flow reactors (COMPABAR)**

G. Heynderickx, I. Nopens

➤ **BOF-GOA: Generic Protocol for the Advanced Simulation of Processes in Chemical and Bio-Science Engineering (PROSIME)**

G. Heynderickx, I. Nopens

➤ **BOF-AOP: Rational design of Acid Base Synergetic Catalysts for Carbon-Carbon bond Formation via Aldol Condensation**

J. Thybaut, P. Van Der Voort

M2dcR2 $\Rightarrow$ Applications in 2013 -not honoured- FP7

➤ *FP7-PEOPLE-2013-IAPP: Unified biomass to refinery (UNIBITOR)*

K. Van Geem, J. Thybaut, G.B. Marin

M2dcR2 $\Rightarrow$ Applications in 2013 -not honoured- IWT

➤ *IWT-FISCH-ATOM*

G. Heynderickx, C. Stevens

M2dcR2 $\Rightarrow$ Applications in 2013 -not honoured- IWT

- *IWT-SBO: Technologies to Convert CO₂ to Chemical Building Blocks (CO₂CHEM) [September 2014]*

K. Rabaey, S. Patil, C. Stevens

M2dcR2 $\Rightarrow$ Applications in 2013 -not honoured- FWO

- *FWO-WOG: Sustainable Chemistry: synthesis of fine chemicals*

C.V. Stevens, J. Thybaut, K. Van Geem, G.B. Marin

- *FWO: Absorption and catalytic kinetics on acid-exchange resins: from experimental insight to fundamental understanding*

J. Thybaut

- *FWO: Pyrolysis of organic waste streams and upgrading to value added products*

K. Van Geem, J. Yperman, R. Carleer, B. Van der Bruggen

M2dcR2 $\Rightarrow$ Applications in 2013 -not honoured- BOF

- **BOF-GOA: Reaction Engineering driving Genetic modification (EDGE)**
M.-F. Reyniers, K. Van Geem, Wout Boerjan, Frederic Lynen, Kris Morreel, Martins José C, John Ralph
- **BOF-GOA: Reactor and Catalyst Design by Microkinetic Modelling: An Integrated Approach for Gas Phase Oxidation (aCaDeMIA-GPO)**
J. Thybaut, G. Heynderickx

M2dcR2 $\Rightarrow$ Applications in 2013 -not honoured- Hercules

- **HERCULES: Synthesis, Operando Characterisation and Reactivity Analysis in an inTegrated Experimental Station (SOCRATES)**

G.B. Marin, Christophe Detavernier, Hilde Poelman, Vladimir Galvita,
J. Thybaut

M2dcR2 $\Rightarrow$ Applications in 2014 -not honoured- H2020

- *H2020-LCE-2014-1: SOLarised Bio-Derived fuels from biomass gasification (SOLBIOD)*

K. Van Geem, G.B. Marin

- *H2020-NMP-2014-two-stage: Materials for Advanced Chemical Coupling in Hypersonic (MAC2H)*

K. Van Geem

- *H2020-NMP-CSA-2014: Raising Awareness on Advanced Nanotechnology & Materials (RANANO)*

J. Thybaut, G.B. Marin

- *H2020-MSCA-IF-2014: Oxidative Coupling of Methane in a Gas-Solid Vortex Reactor (OCM in Vortex)*

A. Obradovic, G.B. Marin

M2dcR2 $\Rightarrow$ Applications in 2014 -not honoured- FWO

- Compact representation of complex polymerisation [March 2014]
D. Constales, D. D'Hooge, M.-F. Reyniers
- *FWO*: Valorization of agricultural waste streams by microwave pyrolysis and upgrading to value added products [March 2014]
S. Schreurs, K. Van Geem

M2dcR2 $\Rightarrow$ Applications in 2014 -not honoured- BOF

- *IOP*: Transgenic hybrid poplar for sustainable production of specialty chemicals

W. Boerjan, K. Van Geem

M2dcR2 $\Rightarrow$ Applications in 2014 -not honoured- Francqui

➤ *FRANCQUI (International Francqui Professor): Rodney Fox*

G.B. Marin

M2dcR2 $\Rightarrow$ Applications in 2015 -not honoured- H2020

- *H2020-MSCA-ITN-2015: CFD for Process Intensification through Reactive Flow Modulation (PRIMO)*

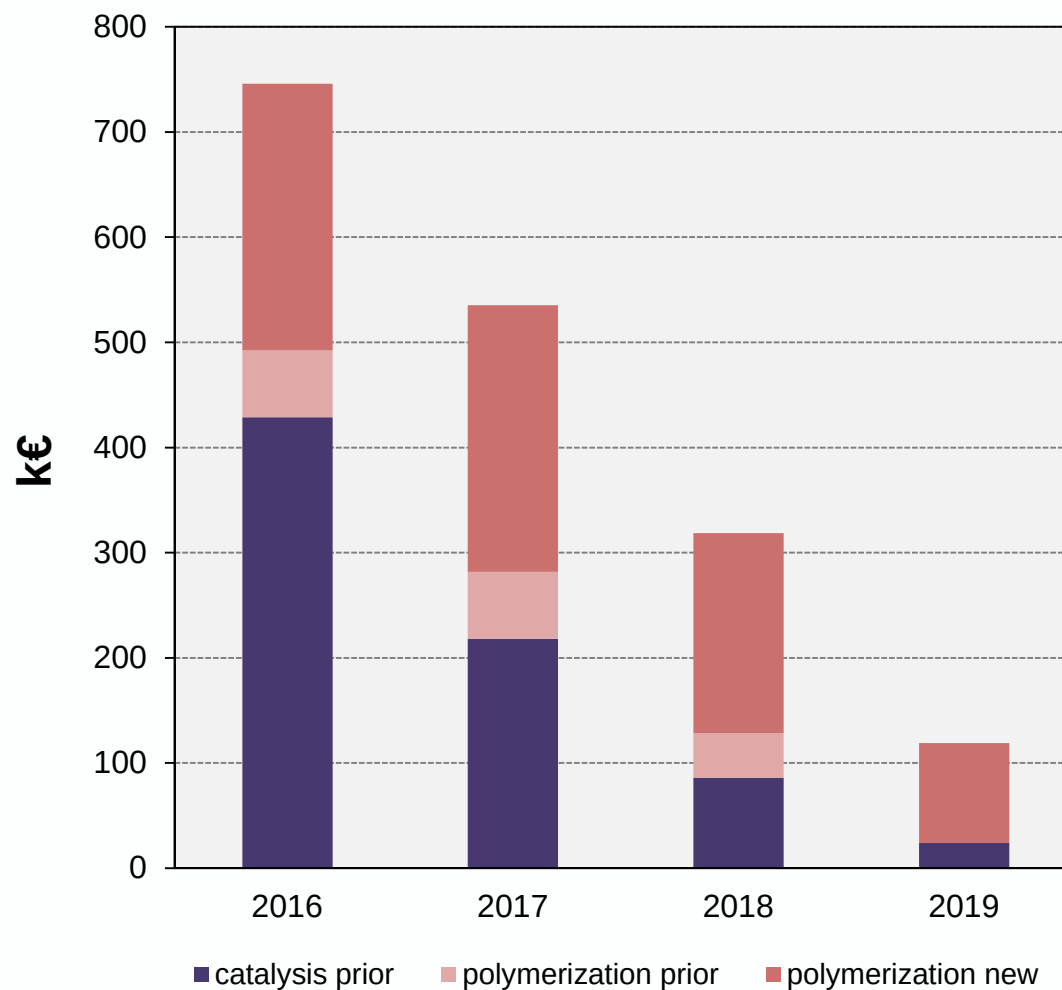
K. Van Geem, G.B. Marin

M2dcR2 $\Rightarrow$ Applications in 2015 -not honoured- H2020

- *IOF-Stepstone: Innovation in Natural Gas Dehydration (SUSTOR2)*
[March 2015]

K. Van Geem, G.B. Marin

Breakdown: polymerization and catalysis



Cumulative: polymerization and catalysis

