

Curriculum vitae Prof. dr. ir. Kevin M. Van Geem

Personal details

Date/place of Birth: July 9, 1977, Ghent, Belgium
 Nationality: Belgian
 Marital Status: Married to Ineke Celie, Master of Chemical Engineering
 Father of Kobe (2010) and Wout (2012)

Affiliation

Laboratory for Chemical Technology, Faculty of Engineering, Ghent University, Belgium

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Professional experience

2017-present Full professor in Thermochemical Reaction Engineering, Ghent University
 Director of the steam cracking pilot plant at LCT, Director of Centre of Sustainable Chemistry (CSC)
 2015-2017 Associate professor in Thermochemical Reaction Engineering, Ghent University
 2010-2015 Assistant professor in Thermochemical Reaction Engineering, Ghent University
 2009- 2010 Fulbright postdoctoral researcher at Massachusetts Institute of Technology (MIT)
 2008- 2009 Postdoctoral researcher at Massachusetts Institute of Technology (MIT)
 2006 - 2009 F.W.O. postdoctoral researcher at LCT, Ghent University
 2002 - 2006 I.W.T Ph.D. fellow at LCT, Ghent University
 2001 ExxonMobil Belgium

Education

2009 Fulbright Post-doctoral researcher, Massachusetts Institute of Technology
 2008 Post-doctoral Researcher, Massachusetts Institute of Technology, Prof. W.H. Green
 2007 F.W.O. Post-doctoral Student, LCT, Ghent University
 2006 Ph.D. in Chemical Engineering, Ghent University, advisor Prof. Guy B. Marin
 2004 Visiting Researcher, Massachusetts Institute of Technology, Prof. W.H. Green
 2001 "Burgerlijk Scheikundig Ingenieur" (Master in Chemical Engineering), Ghent University, magna cum laude

Summary of the scientific output and major achievements up till present (WOS h-index of 21, Scopus: h-index 23):

Publications in WOS: 101 published (17 as first author); 3 accepted, 3 submitted (a detailed list can be found at the end)

5 publications are cited at least 50 times and are published in the most important journals in my field (chemical engineering):

1. *Comprehensive mechanism for combustion and pyrolysis of 1-butanol*
 M.H. Harper, K.M. Van Geem, G.B. Marin, W.H. Green
 Combustion and Flame, 158, 1, 16-41, **2011**, SCI-IF (2011): 3.585, Times Cited: 132
2. *Automatic reaction network generation using RMG for steam cracking of n-hexane*
K.M. Van Geem, M.-F. Reyniers, G.B. Marin, J. Song, D.M. Matheu, W.H. Green
 AIChE Journal, 52 (2): 718-730, **2006**, SCI-IF (2011): 2.261, Times Cited: 58
3. *Effect of radial temperature profiles on yields in steam cracking*
K.M. Van Geem, G.H. Heynderickx, G.B. Marin
 AIChE Journal, 50 (1): 173-183 **2004**, SCI-IF (2011): 2.261, Times Cited: 50
4. *Quantitative analysis of crude and Stabilized bio-oils by comprehensive two-dimensional GC*
 M. Djokic, T.Dijkmans, G. Yildiz, W. Prins, K.M. Van Geem
 Journal of Chromatography A, 1257, 131-140, **2012**, SCI-IF (2011): 4.531, Times Cited: 54
5. *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, 6623-6633, 2010, SCI-IF (2009): 4.101 Times Cited: 50

Books: 2

1. 40 vragen voor 2020
L. Taerwe, H. Romaen, K.M. Van Geem, K. Verbeke
2012, ISBN: 9789020980011 1st and 2nd edition, 296 pages, Publisher: Lannoo
2. Sustainable Chemical Production Processes
K.M. Van Geem and Guy B. Marin
2019, to be published by De Gruyter

Research Group:

Present: promoter of 27 Ph.D. candidates, 13 undergraduate students, 4 postdoctoral researchers

Past: advisor of 9 Ph.D. researchers, 8 postdoctoral researchers, 75 undergraduate students

Presentations at international congresses and in institutes:

103 oral presentations (8 key note presentations) at international conferences and 16 oral presentations at companies.

1. *Genetically modified biomass: effect of single gene modifications on the composition of fast pyrolysis bio-oils.*
K.M. Van Geem, Y. Van Wonterghem, E. Boren, R. Vanholme, L. Gerber, M Djokic, F. Ronsse, W. Prins, B. Sundberg, W. Boerjan, G.B. Marin
AIChE Annual Meeting, Pittsburgh, PA, USA, October 28 - November 1, **2012**
2. *Bio-Ethylene Production: Alternatives for Green Chemicals and Polymers*
K.M. Van Geem, S.P. Pyl, A. Harlin, J.M. Anthonykuty, R. Kaila, G.B. Marin
AIChE Spring Meeting, Houston, TX, USA, 1-5 April, **2012**
3. *Quantitative analysis of fast pyrolysis bio-oils by comprehensive two-dimensional gas chromatography*
K.M. Van Geem, M. Djokic, T. Dijkmans, G. Yildiz, W. Prins, G.B. Marin (*Invited Lecture*)
Twelfth International Symposium on Hyphenated Techniques in Chromatography and Hyphenated Chromatographic Analyzers (HTC-12), Bruges, Belgium, February 1-3, **2012**
4. *Comprehensive 2D GC: the future for analyzing complex fossil and renewable matrices*
K.M. Van Geem (*Invited Lecture*)
Thirteenth International Symposium on Hyphenated Techniques in Chromatography and Hyphenated Chromatographic Analyzers (HTC-13), Bruges, Belgium, January 29 - 31, 2014.
5. *Furnace coils – on-going developments & new applications*
K.M. Van Geem (*invited Lecture*)
EEPC 2015 ETHYLENE SEMINAR
Grandior Hotel – Prague – Czech Republic – 21-23 October 2015
6. *Recent Advances (and continuing challenges) in Biomass fast pyrolysis*
K.M. Van Geem (*KeynoteLecture*)
the 3rd ASEAN Bioenergy Workshop, Hanoi, Vietnam, September 3, 2015

Patents

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Infrastructure

- 1 pilot plant
- 3 bench scale setups
- 6 GCxGC with MS, SCD, NCD, FID

Spin-off

- AVGI, started in 2015, Reaction engineering solutions for the chemical industry

Grants and awards

1. Fulbright scholarship 2009
2. FWO postdoctoral fellowship 2006 (6 years)
3. Travel grant for stays at MIT (3) from FWO, 15000€total, 2004, 2008, 2009
4. IWT research scholarship 2002 (4 years)
5. Laureate Chemistry Olympics, 1995

Educational activities

1. Lecturer for several courses (e.g. **Sustainable Chemical Production Processes**) amounting to an equivalent of 15 ECTS points in the bachelor and master in chemical engineering at Ghent University.
2. Summer and winter courses e.g. (**Fuel me up. The BIO-path to the future!, introduction to reaction engineering**), Ghent, Belgium, 2012 and 2013. TOPCOMBI winter course on: **Design and Optimization of Catalytic Processes: From Laboratory Experiments to Design of Industrial Reactors**, Ghent, Belgium, January 11-15, 2010.

Services to the academic community

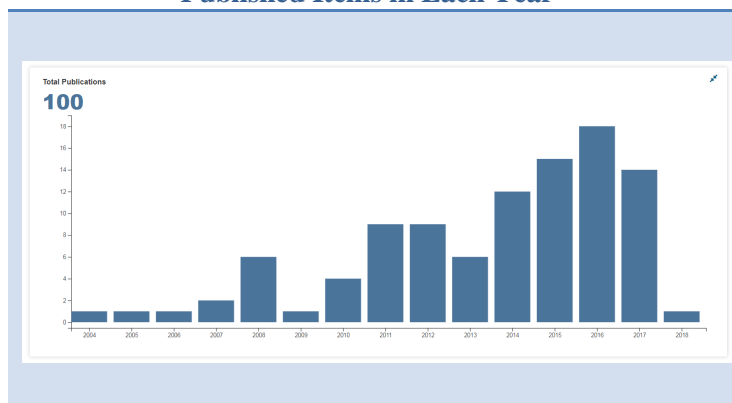
1. Organizer of Chemreactor and MACKIE in Ghent (2018)
2. Organizer of International Conference on Chemical Kinetics (ICCK) in 2013 in Seville and ICCK 2015 in Gent.
3. Member of the Scientific and Organization Committee: International conference on Chemical Kinetics (ICCK 2011), Cambridge, MA, USA, July 10-14, 2011; International conference on Chemical Kinetics (ICCK 2013), Seville, Spain, July 8-12, 2013
4. Referee for more than 30 journals, amongst others several high-impact journals: Chemical Reviews (IF: 40.197); Angewandte Chemie (I.F.: 13.734); Catalysis Reviews (IF: 7.500); Bioresource Technology (IF: 4.987), Combustion and Flame (I.F.: 3.599); etc.
5. Session chair: **'De-Polymerization and Ring-Opening Pyrolysis'** and **'Poster session'** at International conference on Chemical Kinetics (ICCK 2011), Cambridge, Ma, USA, July 10-14, 2011
6. Member of the **COST action CM0901** and **CM1404-SMARTCAT**
7. Member of the Process Engineering for Sustainable Energy section of EFCE
8. External PhD jury member for 9 PhD's: ENSIC Nancy (2), Univ. Orléans (3), Universiteit Hasselt (2), Univ. de Toulouse, TU Delft

Early achievements track-record

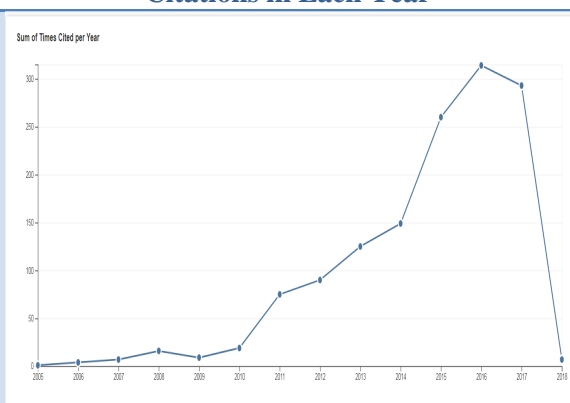
Publications

My research has, so far, resulted in 65 accepted A1 papers out of which 59 date since my PhD. A dozen papers are in press or have been recently submitted for publication. My output in terms of publications has been growing strongly since my appointments as assistant professor, see the figure below. The number of citations of my papers is steadily increasing over the years, currently totaling 725. All this results in an *h-index* of 17. My full bibliography is available at: <https://biblio.ugent.be/person/001995338294>

Published Items in Each Year



Citations in Each Year



Journal	# articles	Impact factor
Industrial and Engineering Chemistry Research	20	2.237
Chemical Engineering Journal	8	3.461
Journal of Chromatography A	5	4.531
Journal of Analytical and Applied Pyrolysis	5	2.487
AIChE Journal	6	2.261
Combustion and Flame	8	3.585
Green chemistry	3	8.020

Computers & Chemical Engineering	3	2.072
Bioresource Technology	2	4.987
Proceedings of the Combustion Institute	2	3.663
Energy	1	3.487
Fuel	2	3.085

I consider my field as “chemical engineering” with a focus on thermal processes using and developing advanced analytical techniques. Both in pyrolysis and chemical analysis I am considered one of the World’s top experts. Chemical engineering has a median impact factor of 1.050 and an aggregate impact factor of 2.158. With an average impact factor of 2.781 I go significantly beyond these figures. It is the result of a publication strategy aiming at the more widespread journals with a high impact factor and not focusing on the number of papers only.

Presentations and organization of international congresses

My total number of presentations at international conferences and workshops amounts to 101 out of which 30 have been presented by myself. I typically present my research at the major conferences within chemical engineering, such as the International Symposium on Chemical Reaction Engineering (ISCRE), the annual and spring meeting of the American Institute of Chemical Engineers (AIChE annual and spring meetings), the International Congress on Chemical Kinetics (ICCK) and at meetings of the American Chemical Society (ACS). I was also one of the organizers and members of scientific committee of the ICCK conference in Cambridge, MA, USA and in Seville (2013). I have been session chair of 7 sessions at these conferences. I am one of the members of the organization/scientific committee.

I have given 5 keynote presentations at international conferences. On 2 occasions this was on the use of biomass for the production of olefins (Chemreactor19, 2010; EEPC, 2010). The other 3 occasions were on the application of 2D comprehensive gas chromatography for processes using fossil and renewable feedstocks (8th GC×GC Symposium, 2010; HTC-12, 2012; HTC-13, 2014).

Invited presentations at research institutes, companies and universities

Although my research is fundamental in nature, e.g. using detailed kinetics and computational chemistry, and I am using conventional and atypical feeds for established processes, e.g. biomass waste streams, I am invited frequently by the major chemical companies to present the research carried out under my guidance. In the period 2011 and 2015 I gave invited lectures at the following universities, companies, and research institutes: East China University of Science and Technology, Tsinghua University, MIT, Politecnico di Milano, CNRS Nancy ExxonMobil, Petrochina, Sinopec, DOW, BASF, SABIC, TOTAL, etc.

Academic collaborations

A broad network of academic collaborations has been established throughout Europe and even worldwide with groups that belong to the top of the World in their specific research area. There has been and is a long lasting cooperation with *Prof. Green (Massachusetts Institute of Technology)* in the field of thermochemical reaction engineering. My membership of the COST action CM0901 on cleaner combustion has intensified collaboration between UGent, **Politecnico di Milano** and **Centre National de la Recherche Scientifique de Nancy** more specific with *Prof. Ranzi (Milano)* and *Prof. Battin-Leclerc (Nancy)*.

There is also a strong interaction with institutes focusing on biomass genetic modification (*Prof. Boerjan* and *Prof. Inzé, Vlaams Instituut voor Biotechnologie*), and on the use of biomass for production of fuels and energy (*Prof. Sels KU Leuven*; *Prof. Harlin, Technical Research Centre of Finland VTT*). My group also belongs to the multidisciplinary partnership Ghent Bio-economy of *Em. Prof. Verstraete* and *Prof. Soetaert*, which creates a lot of interaction within **Ghent University** on the use of biomass.

In the field of compositional modeling my group collaborates with the **University of Delaware** (*Prof. Klein*) and with **IFP-EN** (dr. Verstraete). For GC×GC there was collaboration with the **University of Amsterdam** (*Em. Prof. Beens* and *dr. Blomberg*). For process simulation, control and optimization there is a bilateral scientific cooperation with *Prof. Zhou* and *Prof. Qian* from the UNILAB, State-Key Laboratory of Chemical Engineering, **East China University of Science and Technology (ECUST)** in Shanghai. A recent project on bio-oil purification using metal organic framework was initiated together with *Prof. De Vos (KU Leuven)* funded by Belgian Federal government. Finally for Computational Fluid Dynamics my group collaborates with the group of *Prof. Fox* and *Prof. Passalacqua (Iowa State University)*

Publications included in Web of Science:

1-127

1. Reyniers, P. A.; Vandewalle, L. A.; Saerens, S.; de Smedt, P.; Marin, G. B.; Van Geem, K. M., Techno-economic analysis of an absorption based methanol to olefins recovery section. *Applied Thermal Engineering* **2017**, 115, 477-490.
2. Sarris, S. A.; Olahova, N.; Verbeken, K.; Reyniers, M. F.; Marin, G. B.; Van Geem, K. M., Optimization of the in Situ Pretreatment of High Temperature Ni-Cr Alloys for Ethane Steam Cracking. *Industrial & Engineering Chemistry Research* **2017**, 56, (6), 1424-1438.
3. De Bruycker, R.; Tran, L. S.; Carstensen, H. H.; Glaude, P. A.; Monge, F.; Alzueta, M. U.; Battin-Leclerc, F.; Van Geem, K. M., Experimental and modeling study of the pyrolysis and combustion of 2-methyl-tetrahydrofuran. *Combustion and Flame* **2017**, 176, 409-428.
4. Verhees, P.; Mahulkar, A. V.; Van Geem, K. M.; Heynderickx, G. J., Thermal Fouling of Heat Exchanger Tubes due to Heavy Hydrocarbon Droplets Impingement. *Heat Transfer Engineering* **2017**, 38, (7-8), 712-720.
5. Zhang, Y.; Reyniers, P. A.; Schietekat, C. M.; Van Geem, K. M.; Marin, G. B.; Du, W. L.; Qian, F., Computational fluid dynamics-based steam cracking furnace optimization using feedstock flow distribution. *Aiche Journal* **2017**, 63, (7), 3199-3213.
6. Van Cauwenberge, D. J.; Vandewalle, L. A.; Reyniers, P. A.; Van Geem, K. M.; Marin, G. B.; Flore, J., Periodic Reactive Flow Simulation: Proof of Concept for Steam Cracking Coils. *Aiche Journal* **2017**, 63, (5), 1715-1726.
7. Zhang, Y.; Reyniers, P. A.; Du, W. L.; Qian, F.; Van Geem, K. M.; Marin, G. B., Incident Radiative Heat Flux Based Method for the Coupled Run Length Simulation of Steam Cracking Furnaces. *Industrial & Engineering Chemistry Research* **2017**, 56, (14), 4156-4172.
8. Amghizar, I.; Vandewalle, L. A.; Van Geem, K. M.; Marin, G. B., New Trends in Olefin Production. *Engineering* **2017**, 3, (2), 171-178.
9. Delbeke, E. I. P.; Movsisyan, M.; Van Geem, K. M.; Stevens, C. V., Chemical and enzymatic modification of sophorolipids. *Green Chemistry* **2016**, 18, (1), 76-104.
10. Van de Vijver, R.; Vandewiele, N. M.; Reyniers, M. F.; Marin, G. B.; Van Geem, K. M., Implementation of stereochemistry in automatic kinetic model generation. *International Journal of Chemical Kinetics* **2016**.
11. Negandar, L.; Gonzalez-Quiroga, A.; Otyuskaya, D.; Toraman, H. E.; Liu, L.; Jastrzebski, J.; Van Geem, K. M.; Marin, G. B.; Thybaut, J. W.; Weckhuysen, B. M., Characterization and Comparison of Fast Pyrolysis Bio-oils from Pinewood, Rapeseed Cake, and Wheat Straw Using C-13 NMR and Comprehensive GC x GC. *ACS Sustain. Chem. Eng.* **2016**, 4, (9), 4974-4985.
12. Toraman, H. E.; Vanholme, R.; Borén, E.; Vanwongerghem, Y.; Djokic, M. R.; Yildiz, G.; Ronsse, F.; Prins, W.; Boerjan, W.; Van Geem, K. M.; Marin, G. B., Potential of genetically engineered hybrid poplar for pyrolytic production of bio-based phenolic compounds. *Bioresource Technology* **2016**, 207, 229-236.
13. Ristic, N. D.; Djokic, M. R.; Van Geem, K. M.; Marin, G. B., On-line Analysis of Nitrogen Containing Compounds in Complex Hydrocarbon Matrixes. **2016**, (114), e54236.
14. Olahova, N.; Djokic, M. R.; Van de Vijver, R.; Ristic, N. D.; Marin, G. B.; Reyniers, M.-F.; Van Geem, K. M., Thermal Decomposition of Sulfur Compounds and their Role in Coke Formation during Steam Cracking of Heptane. *Chemical Engineering & Technology* **2016**, 39, (11), 2096-2106.
15. De Bruycker, R.; Amghizar, I.; Vermeire, F. H.; Nyman, T.; Hakola, M.; Van Geem, K. M., Steam cracking of bio-derived normal and branched alkanes: Influence of branching on product distribution and formation of aromatics. *Journal of Analytical and Applied Pyrolysis* **2016**, 122, 468-478.

16. Vargas, D. C.; Alvarez, M. B.; Portilla, A. H.; Van Geem, K. M.; Streitwieser, D. A., Kinetic Study of the Thermal and Catalytic Cracking of Waste Motor Oil to Diesel-like Fuels. *Energy & Fuels* **2016**, 30, (11), 9712-9720.
17. De Bruycker, R.; Herbinet, O.; Carstensen, H. H.; Battin-Leclerc, F.; Van Geem, K. M., Understanding the reactivity of unsaturated alcohols: Experimental and kinetic modeling study of the pyrolysis and oxidation of 3-methyl-2-butenol and 3-methyl-3-butenol. *Combustion and Flame* **2016**, 171, 237-251.
18. Delbeke, E. I. P.; Roelants, S.; Matthijs, N.; Everaert, B.; Soetaert, W.; Coenye, T.; Van Geem, K. M.; Stevens, C. V., Sophorolipid Amine Oxide Production by a Combination of Fermentation Scale-up and Chemical Modification. *Industrial & Engineering Chemistry Research* **2016**, 55, (27), 7273-7281.
19. Delbeke, E. I. P.; Lozach, O.; Le Gall, T.; Berchel, M.; Montier, T.; Jaffres, P. A.; Van Geem, K. M.; Stevens, C. V., Evaluation of the transfection efficacies of quaternary ammonium salts prepared from sophorolipids. *Organic & Biomolecular Chemistry* **2016**, 14, (15), 3744-3751.
20. Van Cauwenberge, D. J.; Vandewalle, L. A.; Reyniers, P. A.; Van Geem, K. M.; Marin, G. B.; Floré, J., Periodic reactive flow simulation: Proof of concept for steam cracking coils. *AIChE Journal* **2016**, n/a-n/a.
21. Olahova, N.; Djokic, M. R.; Van de Vijver, R.; Ristic, N. D.; Marin, G. B.; Reyniers, M. F.; Van Geem, K. M., Thermal Decomposition of Sulfur Compounds and their Role in Coke Formation during Steam Cracking of Heptane. *Chemical Engineering & Technology* **2016**, 39, (11), 2096-2106.
22. Verhees, P.; Amghizar, I.; Goemare, J.; Akhras, A. R.; Marin, G. B.; Van Geem, K. M.; Heynderickx, G. J., 1D Model for Coupled Simulation of Steam Cracker Convection Section with Improved Evaporation Model. *Chemie Ingenieur Technik* **2016**, 88, (11), 1650-1664.
23. Vandewiele, N. M.; Van de Vijver, R.; Carstensen, H. H.; Van Geem, K. M.; Reyniers, M. F.; Marin, G. B., Implementation of Stereochemistry in Automatic Kinetic Model Generation. *International Journal of Chemical Kinetics* **2016**, 48, (12), 755-769.
24. Gonzalez-Quiroga, A.; Djokic, M. R.; Van Geem, K. M.; Marin, G. B., Conversion of Solid Waste to Diesel via Catalytic Pressureless Depolymerization: Pilot Scale Production and Detailed Compositional Characterization. *Energy & Fuels* **2016**, 30, (10), 8292-8303.
25. Reyniers, P. A.; Sarris, S. A.; Marin, G. B.; Van Geem, K. M., Computational Fluid Dynamic Design of Jet Stirred Reactors for Measuring Intrinsic Kinetics of Gas-Phase and Gas-Solid Reactions. *International Journal of Chemical Kinetics* **2016**, 48, (9), 556-569.
26. Toraman, H. E.; Franz, K.; Ronsse, F.; Van Geem, K. M.; Marin, G. B., Quantitative analysis of nitrogen containing compounds in microalgae based bio-oils using comprehensive two-dimensional gas-chromatography coupled to nitrogen chemiluminescence detector and time of flight mass spectrometer. *Journal of Chromatography A* **2016**, 1460, 135-146.
27. Van de Vijver, R.; Devocht, B. R.; Van Geem, K. M.; Thybaut, J. W.; Marin, G. B., Challenges and opportunities for molecule-based management of chemical processes. *Current Opinion in Chemical Engineering* **2016**, 13, 142-149.
28. Toraman, H. E.; Vanholme, R.; Boren, E.; Vanwongerghem, Y.; Djokic, M. R.; Yildiz, G.; Ronsse, F.; Prins, W.; Boerjan, W.; Van Geem, K. M.; Marin, G. B., Potential of genetically engineered hybrid poplar for pyrolytic production of bio-based phenolic compounds. *Bioresource Technology* **2016**, 207, 229-236.
29. Yildiz, G.; Ronsse, F.; Vercruyssen, J.; Daels, J.; Toraman, H. E.; van Geem, K. M.; Marin, G. B.; van Duren, R.; Prins, W., In situ performance of various metal doped catalysts in micro-pyrolysis and continuous fast pyrolysis. *Fuel Processing Technology* **2016**, 144, 312-322.
30. De Bruycker, R.; Carstensen, H. H.; Reyniers, M. F.; Marin, G. B.; Simmie, J. M.; Van Geem, K. M., An experimental and kinetic modeling study of gamma-valerolactone pyrolysis. *Combustion and Flame* **2016**, 164, 183-200.
31. De Bruycker, R.; Simmie, J. M.; Carstensen, H. H.; Van Geem, K. M.; Marin, G. B., Experimental and computational study of the initial decomposition of gamma-valerolactone. *Proceedings of the Combustion Institute* **2015**, 34, (1), 251-258.

32. Delbeke, E. I. P.; Roman, B. I.; Marin, G. B.; Van Geem, K. M.; Stevens, C. V., A new class of antimicrobial biosurfactants: quaternary ammonium sophorolipids. *Green Chemistry* **2015**, 17, (6), 3373-3377.
33. Dijkmans, T.; Djokic, M. R.; Van Geem, K. M.; Marin, G. B., Comprehensive compositional analysis of sulfur and nitrogen containing compounds in shale oil using GC x GC - FID/SCD/NCD/TOF-MS. *Fuel* **2015**, 140, 398-406.
34. Gao, C. W.; Vandeputte, A. G.; Yee, N. W.; Green, W. H.; Bonomi, R. E.; Magoon, G. R.; Wong, H. W.; Oluwole, O. O.; Lewis, D. K.; Vandewiele, N. M.; Van Geem, K. M., JP-10 combustion studied with shock tube experiments and modeled with automatic reaction mechanism generation. *Combustion and Flame* **2015**, 162, (8), 3115-3129.
35. Hu, G. H.; Schietekat, C. M.; Zhang, Y.; Qian, F.; Heynderickx, G.; Van Geem, K. M.; Marin, G. B., Impact of Radiation Models in Coupled Simulations of Steam Cracking Furnaces and Reactors. *Industrial & Engineering Chemistry Research* **2015**, 54, (9), 2453-2465.
36. Van Cauwenberge, D. J.; Schietekat, C. M.; Floré, J.; Van Geem, K. M.; Marin, G. B., CFD-based design of 3D pyrolysis reactors: RANS vs. LES. *Chemical Engineering Journal* **2015**, 282, 66-76.
37. Van de Vijver, R.; Vandewiele, N. M.; Bhoorasingh, P. L.; Slakman, B. L.; Seyedzadeh Khanshan, F.; Carstensen, H.-H.; Reyniers, M.-F.; Marin, G. B.; West, R. H.; Van Geem, K. M., Automatic Mechanism and Kinetic Model Generation for Gas- and Solution-Phase Processes: A Perspective on Best Practices, Recent Advances, and Future Challenges. *International Journal of Chemical Kinetics* **2015**, 47, (4), 199-231.
38. Van de Vijver, R.; Vandewiele, N. M.; Vandeputte, A. G.; Van Geem, K. M.; Reyniers, M.-F.; Green, W. H.; Marin, G. B., Rule-based ab initio kinetic model for alkyl sulfide pyrolysis. *Chemical Engineering Journal* **2015**, 278, (0), 385-393.
39. Vandewiele, N. M.; Magoon, G. R.; Van Geem, K. M.; Reyniers, M. F.; Green, W. H.; Marin, G. B., Kinetic Modeling of Jet Propellant-10 Pyrolysis. *Energy & Fuels* **2015**, 29, (1), 413-427.
40. Vandewiele, N. M.; Van de Vijver, R.; Van Geem, K. M.; Reyniers, M. F.; Marin, G. B., Symmetry calculation for molecules and transition states. *J Comput Chem* **2015**, 36, (3), 181-92.
41. Zhang, Y.; Qian, F.; Zhang, Y.; Schietekat, C. M.; Van Geem, K. M.; Marin, G. B., Impact of Flue Gas Radiative Properties and Burner Geometry in Furnace Simulations. *Aiche Journal* **2015**, 61, (3), 936-954.
42. Reyniers, P. A.; Schietekat, C. M.; Van Cauwenberge, D. J.; Vandewalle, L. A.; Van Geem, K. M.; Marin, G. B., Necessity and Feasibility of 3D Simulations of Steam Cracking Reactors. *Industrial & Engineering Chemistry Research* **2015**, 54, (49), 12270-12282.
43. Schietekat, C. M.; Sarris, S. A.; Reyniers, P. A.; Kool, L. B.; Peng, W. Q.; Lucas, P.; Van Geem, K. M.; Marin, G. B., Catalytic Coating for Reduced Coke Formation in Steam Cracking Reactors. *Industrial & Engineering Chemistry Research* **2015**, 54, (39), 9525-9535.
44. De Bruycker, R.; Carstensen, H.-H.; Simmie, J. M.; Van Geem, K. M.; Marin, G. B., Experimental and computational study of the initial decomposition of gamma-valerolactone. *Proceedings of the Combustion Institute* **2015**, 35, (1), 515-523.
45. Van Geem, K. M., *Sustainable chemical production processes*. 2014.
46. Mahulkar, A. V.; Heynderickx, G. J.; Marin, G. B., Simulation of the coking phenomenon in the superheater of a steam cracker. *Chemical Engineering Science* **2014**, 110, 31-43.
47. De Bruycker, R.; Anthonykutty, J. M.; Linnekoski, J.; Harlin, A.; Lehtonen, J.; Van Geem, K. M.; Räsänen, J.; Marin, G. B., Assessing the Potential of Crude Tall Oil for the Production of Green-Base Chemicals: An Experimental and Kinetic Modeling Study. *Industrial & Engineering Chemistry Research* **2014**, 53, (48), 18430-18442.
48. Dijkmans, T.; Schietekat, C. M.; Van Geem, K. M.; Marin, G. B., GPU based simulation of reactive mixtures with detailed chemistry in combination with tabulation and an analytical Jacobian. *Computers & Chemical Engineering* **2014**, 71, (0), 521-531.
49. Dijkmans, T.; Van Geem, K. M.; Djokic, M. R.; Marin, G. B., Combined Comprehensive Two-Dimensional Gas Chromatography Analysis of Polyaromatic Hydrocarbons/Polyaromatic

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