Kevin Marcel Van Geem

List of Publications by Year in Descending Order

238 papers	5,957 citations	41 h-index	68 g-index
252 ext. papers	7,837 ext. citations	6.2 avg, IF	6.47 L-index

#	Paper	IF	Citations
238	Detailed Kinetic Modeling for the Pyrolysis of a Jet A Surrogate. *Energy & Fuels*, **2022**, 36, 1304-1315	4.1	2
237	Assessing the feasibility of chemical recycling via steam cracking of untreated plastic waste pyrolysis oils: Feedstock impurities, product yields and coke formation.. *Waste Management*, **2022**, 141, 104-114	8.6	4
236	Analytics Driving Kinetics: Advanced Mass Spectrometric Characterization of Petroleum Products. *Energy & Fuels*, **2022**, 36, 6-59	4.1	0
235	Study of the degradation of epoxy resins used in spacecraft components by thermogravimetry and fast pyrolysis. *Journal of Analytical and Applied Pyrolysis*, **2022**, 161, 105397	6	1
234	A comprehensive experimental investigation of plastic waste pyrolysis oil quality and its dependence on the plastic waste composition. *Fuel Processing Technology*, **2022**, 227, 107090	7.2	13
233	Expanding the collection portfolio of plastic packaging: Impact on quantity and quality of sorted plastic waste fractions. *Resources, Conservation and Recycling*, **2022**, 178, 106025	11.9	2
232	Identification and quantification of lignin monomers and oligomers from reductive catalytic fractionation of pine wood with GC GC FID/MS. *Green Chemistry*, **2022**, 24, 191-206	10	9
231	A detailed experimental and kinetic modeling study on pyrolysis and oxidation of oxymethylene ether-2 (OME-2). *Combustion and Flame*, **2022**, 238, 111914	5.3	2
230	Maximizing light olefins and aromatics as high value base chemicals via single step catalytic conversion of plastic waste. *Chemical Engineering Journal*, **2022**, 428, 132087	14.7	9
229	Speeding up turbulent reactive flow simulation via a deep artificial neural network: A methodology study. *Chemical Engineering Journal*, **2022**, 429, 132442	14.7	2
228	Combined Catalytic and Pyrolytic Coking Model for Steam Cracking of Hydrocarbons. *Industrial & Engineering Chemistry Research*, **2022**, 61, 3917-3927	3.9	3
227	Removal of volatile components from plastic waste in liquid media: effect of temperature and particle size. *Resources, Conservation and Recycling*, **2022**, 106267	11.9	2
226	Statistical entropy of resources using a categorization tree for material enumeration: Framework development and application to a plastic packaging case study. *Resources, Conservation and Recycling*, **2022**, 181, 106259	11.9	
225	Mixture effects in alkane/cycloalkane hydroconversion over Pt/HUSY: Carbon number impact. *Fuel*, **2022**, 318, 123651	7.1	
224	Analysis of the kinetics, energy balance and carbon footprint of the delamination of multilayer flexible packaging films via carboxylic acids. *Resources, Conservation and Recycling*, **2022**, 181, 106256	11.9	0
223	Highly selective conversion of mixed polyolefins to valuable base chemicals using phosphorus-modified and steam-treated mesoporous HZSM-5 zeolite with minimal carbon footprint. *Applied Catalysis B: Environmental*, **2022**, 309, 121251	21.8	1
222	CFD analysis on hydrodynamics and residence time distribution in a gas-liquid vortex unit. *Chemical Engineering Journal*, **2022**, 136812	14.7	2

221	Reducing CO2 emissions of existing ethylene plants: Evaluation of different revamp strategies to reduce global CO2 emission by 100 million tonnes. *Journal of Cleaner Production*, **2022**, 132127	10.3	0
220	Maximizing olefin production via steam cracking of distilled pyrolysis oils from difficult-to-recycle municipal plastic waste and marine litter. *Science of the Total Environment*, **2022**, 838, 156092	10.2	2
219	Gas-solid hydrodynamics in a stator-rotor vortex chamber reactor. *Chemical Engineering Journal*, **2022**, 137323	14.7	0
218	Fast pyrolysis of polyurethanes and polyisocyanurate with and without flame retardant: Compounds of interest for chemical recycling. *Journal of Analytical and Applied Pyrolysis*, **2021**, 160, 105374	6	2
217	Opportunities and challenges for the application of post-consumer plastic waste pyrolysis oils as steam cracker feedstocks: To decontaminate or not to decontaminate?. *Waste Management*, **2021**, 138, 83-115	8.6	11
216	Pyrolysis of end-of-life polystyrene in a pilot-scale reactor: Maximizing styrene production.. *Waste Management*, **2021**, 139, 85-95	8.6	5
215	Deodorization of post-consumer plastic waste fractions: A comparison of different washing media.. *Science of the Total Environment*, **2021**, 812, 152467	10.2	5
214	Boron-Modified Mesoporous ZSM-5 for the Conversion of Pyrolysis Vapors from LDPE and Mixed Polyolefins: Maximizing the C2−4 Olefin Yield with Minimal Carbon Footprint. *ACS Sustainable Chemistry and Engineering*, **2021**, 9, 14618-14630	8.3	4
213	Solids lateral mixing and compartmentalization in dynamically structured gas–solid fluidized beds. *Chemical Engineering Journal*, **2021**, 430, 133063	14.7	0
212	Micromixing in a gas–liquid vortex reactor. *AICHE Journal*, **2021**, 67, e17264	3.6	7
211	Endocrine disrupting potency and toxicity of novel sophorolipid quaternary ammonium salts. *Ecotoxicology*, **2021**, 30, 658-666	2.9	1
210	Molecular Reconstruction of Hydrocarbons and Sulfur-Containing Compounds in Atmospheric and Vacuum Gas Oils. *Energy & Fuels*, **2021**, 35, 5777-5788	4.1	2
209	The chemistry of chemical recycling of solid plastic waste via pyrolysis and gasification: State-of-the-art, challenges, and future directions. *Progress in Energy and Combustion Science*, **2021**, 84, 100901	33.6	78
208	Learning Molecular Representations for Thermochemistry Prediction of Cyclic Hydrocarbons and Oxygenates. *Journal of Physical Chemistry A*, **2021**, 125, 5166-5179	2.8	2
207	From 3D to 1D: Capturing the effect of particle clusters in downers in the fluid catalytic cracking of gasoil. *Chemical Engineering Research and Design*, **2021**, 170, 366-379	5.5	
206	Development of Lignin-Based Mesoporous Carbons for the Adsorption of Humic Acid. *ACS Omega*, **2021**, 6, 15222-15235	3.9	3
205	Biomass fast pyrolysis in an innovative gas-solid vortex reactor: Experimental proof of concept. *Journal of Analytical and Applied Pyrolysis*, **2021**, 156, 105165	6	9
204	Primary Thermal Decomposition Pathways of Hydroxycinnamaldehydes. *Energy & Fuels*, **2021**, 35, 12216-12226	4.1	3

203	Effect of Newly Synthesized Salts and Three Common Micropollutants on the Biochemical Activity of Nitrifiers. *Sustainability*, **2021**, 13, 7417	3.6	
202	Detailed Group-Type Characterization of Plastic-Waste Pyrolysis Oils: By Comprehensive Two-Dimensional Gas Chromatography Including Linear, Branched, and Di-Olefins. *Separations*, **2021**, 8, 103	3.1	8
201	Techno-economic assessment of mechanical recycling of challenging post-consumer plastic packaging waste. *Resources, Conservation and Recycling*, **2021**, 170, 105607	11.9	22
200	On the primary thermal decomposition pathways of hydroxycinnamic acids. *Proceedings of the Combustion Institute*, **2021**, 38, 4207-4214	5.9	6
199	Combustion of ethylamine, dimethylamine and diethylamine: Theoretical and kinetic modeling study. *Proceedings of the Combustion Institute*, **2021**, 38, 585-592	5.9	2
198	Thermal decomposition of furans with oxygenated substituents: A combined experimental and quantum chemical study. *Proceedings of the Combustion Institute*, **2021**, 38, 699-707	5.9	3
197	catchyFOAM: EulerEuler CFD Simulations of Fluidized Bed Reactors with Microkinetic Modeling of Gas-Phase and Catalytic Surface Chemistry. *Energy & Fuels*, **2021**, 35, 2545-2561	4.1	7
196	Development and application of a predictive modelling approach for household packaging waste flows in sorting facilities. *Waste Management*, **2021**, 120, 290-302	8.6	24
195	Bond additivity corrections for CBS-QB3 calculated standard enthalpies of formation of H, C, O, N, and S containing species. *International Journal of Chemical Kinetics*, **2021**, 53, 345-355	1.4	2
194	Towards a better understanding of odor removal from post-consumer plastic film waste: A kinetic study on deodorization efficiencies with different washing media. *Waste Management*, **2021**, 120, 564-575	8.6	10
193	Reuse of CO in energy intensive process industries. *Chemical Communications*, **2021**, 57, 10967-10982	5.8	10
192	Determination of heat capacity of carbon composites with application to carbon/phenolic ablators up to high temperatures. *Aerospace Science and Technology*, **2021**, 108, 106375	4.9	6
191	An assessment of electrified methanol production from an environmental perspective. *Green Chemistry*, **2021**, 23, 7243-7258	10	6
190	A Boudart Number for the Assessment of Irreducible Pellet-Scale Mass Transfer Limitations: Application to Oxidative Coupling of Methane. *Industrial & Engineering Chemistry Research*, **2021**, 60, 6538-6553	3.9	3
189	The Effect of Refractory Wall Emissivity on the Energy Efficiency of a Gas-Fired Steam Cracking Pilot Unit. *Materials*, **2021**, 14,	3.5	1
188	Towards a Better Understanding of Delamination of Multilayer Flexible Packaging Films by Carboxylic Acids. *ChemSusChem*, **2021**, 14, 4198-4213	8.3	8
187	Machine Learning in Chemical Engineering: Strengths, Weaknesses, Opportunities, and Threats. *Engineering*, **2021**, 7, 1201-1201	9.7	15
186	Fast screening of Depolymerized Lignin Samples Through 2D-Liquid Chromatography Mapping. *ChemistryOpen*, **2021**, 10, 740-747	2.3	1

185	CFD-based assessment of steady-state multiplicity in a gas-solid vortex reactor for oxidative coupling of methane. *Chemical Engineering and Processing: Process Intensification*, **2021**, 165, 108434	3.7	5
184	Fluid catalytic co-processing of bio-oils with petroleum intermediates: Comparison of vapour phase low pressure hydrotreating and catalytic cracking as pretreatment. *Fuel*, **2021**, 302, 121198	7.1	6
183	Hydrocracking of complex mixtures: From bulk properties, over fundamental kinetics to detailed product composition. *Catalysis Today*, **2021**, 378, 189-201	5.3	0
182	Detailed characterization of sulfur compounds in fast pyrolysis bio-oils using GC GC-SCD and GC MS. *Journal of Analytical and Applied Pyrolysis*, **2021**, 159, 105288	6	2
181	The pyrolysis of oak with polyethylene, polypropylene and polystyrene using fixed bed and stirred reactors and TGA instrument. *Energy*, **2021**, 232, 121085	7.9	4
180	Feasibility of biogas and oxy-fuel combustion in steam cracking furnaces: Experimental and computational study. *Fuel*, **2021**, 304, 121393	7.1	6
179	Decomposition of carbon/phenolic composites for aerospace heatshields: Detailed speciation of phenolic resin pyrolysis products. *Aerospace Science and Technology*, **2021**, 119, 107079	4.9	8
178	Fast estimation of standard enthalpy of formation with chemical accuracy by artificial neural network correction of low-level-of-theory ab initio calculations. *Chemical Engineering Journal*, **2021**, 426, 131304	14.7	2
177	Intensifying Mass and Heat Transfer using a High-g Stator-Rotor Vortex Chamber. *Chemical Engineering and Processing: Process Intensification*, **2021**, 169, 108638	3.7	1
176	Liquid hydrodynamics in a gas-liquid vortex reactor. *Chemical Engineering Science*, **2021**, 246, 116970	4.4	2
175	Distribution Changes during Thermal Degradation of Poly(styrene peroxide) by Pairing Tree-Based Kinetic Monte Carlo and Artificial Intelligence Tools. *Industrial & Engineering Chemistry Research*, **2021**, 60, 3334-3353	3.9	5
174	Computational fluid dynamics-based optimization of dimpled steam cracking reactors for reduced CO2 emissions. *AICHE Journal*, **2020**, 66, e16255	3.6	4
173	Experimental and kinetic modeling study of the pyrolysis and oxidation of diethylamine. *Fuel*, **2020**, 275, 117744	7.1	6
172	Reactor Engineering Aspects of the Lateral Flow Reactor. *Industrial & Engineering Chemistry Research*, **2020**, 59, 11157-11169	3.9	0
171	Dimples in turbulent pipe flows: experimental aero-thermal investigation. *International Journal of Heat and Mass Transfer*, **2020**, 157, 119925	4.9	1
170	Alumina-based Coating for Coke Reduction in Steam Crackers. *Materials*, **2020**, 13,	3.5	3
169	Experimental and theoretical study of the thermal decomposition of ethyl acetate during fast pyrolysis. *Chemical Engineering Research and Design*, **2020**, 157, 153-161	5.5	7
168	Artificial Intelligence for Computer-Aided Synthesis In Flow: Analysis and Selection of Reaction Components. *Frontiers in Chemical Engineering*, **2020**, 2,	1	7

167	Crude to Olefins: Effect of Feedstock Composition on Coke Formation in a Bench-Scale Steam Cracking Furnace. *Industrial & Engineering Chemistry Research*, **2020**, 59, 2849-2859	3.9	4
166	Monometallic Cerium Layered Double Hydroxide Supported Pd-Ni Nanoparticles as High Performance Catalysts for Lignin Hydrogenolysis. *Materials*, **2020**, 13,	3.5	2
165	Challenges and opportunities of solvent-based additive extraction methods for plastic recycling. *Waste Management*, **2020**, 104, 148-182	8.6	60
164	Hydrodynamic analysis of an axial impeller in a non-Newtonian fluid through particle image velocimetry. *AICHE Journal*, **2020**, 66, e16939	3.6	5
163	Microstructural Contributions of Different Polyolefins to the Deformation Mechanisms of Their Binary Blends. *Polymers*, **2020**, 12,	4.5	11
162	Steam Cracking Coke Properties and Their Influence on Furnace Run Length Predictions: Experimental and Modeling Study. *Industrial & Engineering Chemistry Research*, **2020**, 59, 22460-22472	3.9	1
161	The role of chemistry in the oscillating combustion of hydrocarbons: An experimental and theoretical study. *Chemical Engineering Journal*, **2020**, 385, 123401	14.7	12
160	A multi-layered view of chemical and biochemical engineering. *Chemical Engineering Research and Design*, **2020**, 155, A133-A145	5.5	43
159	Sustainable innovations in steam cracking: CO2 neutral olefin production. *Reaction Chemistry and Engineering*, **2020**, 5, 239-257	4.9	24
158	Influence of obstacles on the wall heat transfer for 2D and 3D helically ribbed pipes. *International Journal of Heat and Mass Transfer*, **2020**, 148, 119087	4.9	1
157	Detailed Analysis of the Composition of Selected Plastic Packaging Waste Products and Its Implications for Mechanical and Thermochemical Recycling. *Environmental Science & Technology*, **2020**, 54, 13282-13293	10.3	60
156	Detailed experimental and kinetic modeling study of 3-carene pyrolysis. *International Journal of Chemical Kinetics*, **2020**, 52, 785-795	1.4	2
155	Progress in Reaction Mechanisms and Reactor Technologies for Thermochemical Recycling of Poly(methyl methacrylate). *Polymers*, **2020**, 12,	4.5	27
154	Towards closed-loop recycling of multilayer and coloured PET plastic waste by alkaline hydrolysis. *Green Chemistry*, **2020**, 22, 5376-5394	10	67
153	Connecting polymer synthesis and chemical recycling on a chain-by-chain basis: a unified matrix-based kinetic Monte Carlo strategy. *Reaction Chemistry and Engineering*, **2020**, 5, 1909-1928	4.9	25
152	Catalytic Effect of Dimethyl Disulfide on Coke Formation on High-Temperature Alloys: Myth or Reality?. *Industrial & Engineering Chemistry Research*, **2020**, 59, 15165-15178	3.9	2
151	Fouling in a Steam Cracker Convection Section Part 1: A Hybrid CFD-1D Model to Obtain Accurate Tube Wall Temperature Profiles. *Heat Transfer Engineering*, **2020**, 41, 127-137	1.7	3
150	Fouling in a Steam Cracker Convection Section Part 2: Coupled Tube Bank Simulation using an Improved Hybrid CFD-1D Model. *Heat Transfer Engineering*, **2020**, 41, 1531-1551	1.7	1

149	Large eddy simulation of tubular reactors with spherical dimples. *Chemical Engineering Journal*, **2020**, 380, 122463	14.7	4
148	Pyrometer-based control of a steam cracking furnace. *Chemical Engineering Research and Design*, **2020**, 153, 380-390	5.5	4
147	Effects of 2-D and 3-D helical inserts on the turbulent flow in pipes. *Experimental Thermal and Fluid Science*, **2020**, 110, 109923	3	5
146	Evaluation of a Ti-Base Alloy as Steam Cracking Reactor Material. *Materials*, **2019**, 12,	3.5	3
145	Process Intensification in a Gas–Solid Vortex Unit: Computational Fluid Dynamics Model Based Analysis and Design. *Industrial & Engineering Chemistry Research*, **2019**, 58, 12751-12765	3.9	8
144	Azimuthal and radial flow patterns of 1g-Geldart B-type particles in a gas-solid vortex reactor. *Powder Technology*, **2019**, 354, 410-422	5.2	6
143	Kinetic modeling of the pyrolysis chemistry of fossil and alternative feedstocks. *Computer Aided Chemical Engineering*, **2019**, 295-362	0.6	3
142	Making chemicals with electricity. *Science*, **2019**, 364, 734-735	33.3	53
141	Lipid-Based Quaternary Ammonium Sophorolipid Amphiphiles with Antimicrobial and Transfection Activities. *ChemSusChem*, **2019**, 12, 3642-3653	8.3	11
140	Phenolics isolation from bio-oil using the metal-organic framework MIL-53(Al) as a highly selective adsorbent. *Chemical Communications*, **2019**, 55, 6245-6248	5.8	3
139	Asymmetrical, Symmetrical, Divalent, and Y-Shaped (Bola)amphiphiles: The Relationship between the Molecular Structure and Self-Assembly in Amino Derivatives of Sophorolipid Biosurfactants. *Journal of Physical Chemistry B*, **2019**, 123, 3841-3858	3.4	14
138	An experimental and numerical study of the suppression of jets, counterflow, and backflow in vortex units. *AICHE Journal*, **2019**, 65, e16614	3.6	9
137	Analytical Py-GC/MS of Genetically Modified Poplar for the Increased Production of Bio-aromatics. *Computational and Structural Biotechnology Journal*, **2019**, 17, 599-610	6.8	3
136	Geminal Coordinatively Unsaturated Sites on MOF-808 for the Selective Uptake of Phenolics from a Real Bio-Oil Mixture. *ChemSusChem*, **2019**, 12, 1256-1266	8.3	20
135	On-the-fly ab initio calculations toward accurate rate coefficients. *Proceedings of the Combustion Institute*, **2019**, 37, 283-290	5.9	13
134	The thermal decomposition of furfural: molecular chemistry unraveled. *Proceedings of the Combustion Institute*, **2019**, 37, 445-452	5.9	10
133	Artificial Intelligence in Steam Cracking Modeling: A Deep Learning Algorithm for Detailed Effluent Prediction. *Engineering*, **2019**, 5, 1027-1040	9.7	25
132	QUANTIS: Data quality assessment tool by clustering analysis. *International Journal of Chemical Kinetics*, **2019**, 51, 872-885	1.4	3

131	Carbon capture and utilization in the steel industry: challenges and opportunities for chemical engineering. *Current Opinion in Chemical Engineering*, **2019**, 26, 81-87	5.4	29
130	Catalyst ignition and extinction: A microkinetics-based bifurcation study of adiabatic reactors for oxidative coupling of methane. *Chemical Engineering Science*, **2019**, 199, 635-651	4.4	17
129	Methane reforming to valuable products by an atmospheric pressure direct current discharge. *Journal of Cleaner Production*, **2019**, 209, 655-664	10.3	9
128	Measuring biomass fast pyrolysis kinetics: State of the art. *Wiley Interdisciplinary Reviews: Energy and Environment*, **2019**, 8, e326	4.7	27
127	The role of mass and heat transfer in the design of novel reactors for oxidative coupling of methane. *Chemical Engineering Science*, **2019**, 198, 268-289	4.4	30
126	Evaluation of biological properties and fate in the environment of a new class of biosurfactants. *Chemosphere*, **2018**, 200, 561-568	8.4	5
125	Detailed Experimental and Kinetic Modeling Study of Cyclopentadiene Pyrolysis in the Presence of Ethene. *Energy & Fuels*, **2018**, 32, 3920-3934	4.1	15
124	Coking Tendency of 25Cr-35Ni Alloys: Influence of Temperature, Sulfur Addition, and Cyclic Aging. *Industrial & Engineering Chemistry Research*, **2018**, 57, 3138-3148	3.9	9
123	Automated reaction database and reaction network analysis: extraction of reaction templates using cheminformatics. *Journal of Cheminformatics*, **2018**, 10, 11	8.6	17
122	Ab initio derived group additivity model for intramolecular hydrogen abstraction reactions. *Physical Chemistry Chemical Physics*, **2018**, 20, 10877-10894	3.6	7
121	A model of tetrahydrofuran low-temperature oxidation based on theoretically calculated rate constants. *Combustion and Flame*, **2018**, 191, 252-269	5.3	23
120	Application of Py-GC/MS coupled with PARAFAC2 and PLS-DA to study fast pyrolysis of genetically engineered poplars. *Journal of Analytical and Applied Pyrolysis*, **2018**, 129, 101-111	6	7
119	Experimental and modeling study of the pyrolysis and combustion of dimethoxymethane. *Combustion and Flame*, **2018**, 190, 270-283	5.3	51
118	CoatAlloy Barrier Coating for Reduced Coke Formation in Steam Cracking Reactors: Experimental Validation and Simulations. *Industrial & Engineering Chemistry Research*, **2018**, 57, 897-907	3.9	10
117	Compositional Characterization of Pyrolysis Fuel Oil from Naphtha and Vacuum Gas Oil. *Energy & Fuels*, **2018**, 32, 1276-1286	4.1	10
116	Upgrading the value of anaerobic digestion via chemical production from grid injected biomethane. *Energy and Environmental Science*, **2018**, 11, 1788-1802	35.4	64
115	Pressure dependent kinetic analysis of pathways to naphthalene from cyclopentadienyl recombination. *Combustion and Flame*, **2018**, 187, 247-256	5.3	42
114	Sophorolipid Modification: The Power of Yeasts and Enzymes **2018**, 315-341		1

113	Computational Fluid Dynamics-Assisted Process Intensification Study for Biomass Fast Pyrolysis in a Gas□Solid Vortex Reactor. *Energy & Fuels*, **2018**, 32, 10169-10183	4.1	21
112	Numerical and experimental evaluation of heat transfer in helically corrugated tubes. *AICHE Journal*, **2018**, 64, 1702-1713	3.6	14
111	Computational Fluid Dynamics-Based Study of a High Emissivity Coil Coating in an Industrial Steam Cracker. *Industrial & Engineering Chemistry Research*, **2018**, 57, 16782-16794	3.9	6
110	Effect of Long-Term High Temperature Oxidation on the Coking Behavior of Ni-Cr Superalloys. *Materials*, **2018**, 11,	3.5	8
109	Combined characterization using HT-GC□GC-FID and FT-ICR MS: A pyrolysis fuel oil case study. *Fuel Processing Technology*, **2018**, 182, 15-25	7.2	10
108	Impact of a Helical Ridge within a Tubular Membrane Channel on Fluid Flow and Particle Behavior: A Model-Based Analysis. *Industrial & Engineering Chemistry Research*, **2018**,	3.9	
107	State-of-the-art of Coke Formation during Steam Cracking: Anti-Coking Surface Technologies. *Industrial & Engineering Chemistry Research*, **2018**, 57, 16117-16136	3.9	32
106	Prediction of the PIONA and oxygenate composition of unconventional fuels with the Pseudo-Component Property Estimation (PCPE) method. Application to an Automotive Shredder Residues-derived gasoline **2018**,		3
105	Synthesis and Biological Evaluation of Bolaamphiphilic Sophorolipids. *ACS Sustainable Chemistry and Engineering*, **2018**, 6, 8992-9005	8.3	14
104	Experimental and Kinetic Modeling Study of Cyclohexane Pyrolysis. *Energy & Fuels*, **2018**, 32, 7153-7168	4.6	7
103	Decomposition and isomerization of 1-pentanol radicals and the pyrolysis of 1-pentanol. *Combustion and Flame*, **2018**, 196, 500-514	5.3	13
102	Periodic reactive flow simulation: Proof of concept for steam cracking coils. *AICHE Journal*, **2017**, 63, 1715-1726	3.6	12
101	Techno-economic analysis of an absorption based methanol to olefins recovery section. *Applied Thermal Engineering*, **2017**, 115, 477-490	5.8	9
100	Optimization of the in Situ Pretreatment of High Temperature Ni□Cr Alloys for Ethane Steam Cracking. *Industrial & Engineering Chemistry Research*, **2017**, 56, 1424-1438	3.9	22
99	Computational fluid dynamics-based steam cracking furnace optimization using feedstock flow distribution. *AICHE Journal*, **2017**, 63, 3199-3213	3.6	9
98	Comprehensive two-dimensional gas chromatography in combination with pixel-based analysis for fouling tendency prediction. *Journal of Chromatography A*, **2017**, 1501, 89-98	4.5	7
97	Quantitative on-line analysis of sulfur compounds in complex hydrocarbon matrices. *Journal of Chromatography A*, **2017**, 1509, 102-113	4.5	13
96	New Trends in Olefin Production. *Engineering*, **2017**, 3, 171-178	9.7	320

95	Design and cold flow testing of a Gas-Solid Vortex Reactor demonstration unit for biomass fast pyrolysis. *Chemical Engineering Journal*, **2017**, 329, 198-210	14.7	37
94	Legal, Social, Ethical, and Medical Perspectives on the Care of the Statutory Rape Adolescent in the Emergency Department. *Annals of Emergency Medicine*, **2017**, 70, 72-79	2.1	1
93	Incident Radiative Heat Flux Based Method for the Coupled Run Length Simulation of Steam Cracking Furnaces. *Industrial & Engineering Chemistry Research*, **2017**, 56, 4156-4172	3.9	7
92	Towards first-principles based kinetic modeling of biomass fast pyrolysis. *Biomass Conversion and Biorefinery*, **2017**, 7, 305-317	2.3	19
91	Experimental and modeling study of the pyrolysis and combustion of 2-methyl-tetrahydrofuran. *Combustion and Flame*, **2017**, 176, 409-428	5.3	21
90	Group additive modeling of cyclopentane pyrolysis. *Journal of Analytical and Applied Pyrolysis*, **2017**, 128, 437-450	6	10
89	Impact of Initial Surface Roughness and Aging on Coke Formation during Ethane Steam Cracking. *Industrial & Engineering Chemistry Research*, **2017**, 56, 12495-12507	3.9	8
88	Quantitative compositional analysis of Estonian shale oil using comprehensive two dimensional gas chromatography. *Fuel Processing Technology*, **2017**, 167, 241-249	7.2	23
87	Experimental and kinetic modeling study of the pyrolysis and oxidation of 1,5-hexadiene: The reactivity of allylic radicals and their role in the formation of aromatics. *Fuel*, **2017**, 208, 779-790	7.1	14
86	Mechanical and chemical recycling of solid plastic waste. *Waste Management*, **2017**, 69, 24-58	8.6	858
85	CFD simulations of Industrial Steam Cracking Reactors: Turbulence Chemistry Interaction and Dynamic Zoning. *Industrial & Engineering Chemistry Research*, **2017**, 56, 14959-14971	3.9	5
84	Dynamic simulation of fouling in steam cracking reactors using CFD. *Chemical Engineering Journal*, **2017**, 329, 77-87	14.7	13
83	Thermal Fouling of Heat Exchanger Tubes due to Heavy Hydrocarbon Droplets Impingement. *Heat Transfer Engineering*, **2017**, 38, 712-720	1.7	4
82	IMPROOF: Integrated Model Guided Process Optimization of Steam Cracking Furnaces. *Smart Innovation, Systems and Technologies*, **2017**, 589-600	0.5	2
81	Conversion of Solid Waste to Diesel via Catalytic Pressureless Depolymerization: Pilot Scale Production and Detailed Compositional Characterization. *Energy & Fuels*, **2016**, 30, 8292-8303	4.1	9
80	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, 135-46	4.5	30
79	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	6	3
78	Kinetic Study of the Thermal and Catalytic Cracking of Waste Motor Oil to Diesel-like Fuels. *Energy & Fuels*, **2016**, 30, 9712-9720	4.1	10

77	1D Model for Coupled Simulation of Steam Cracker Convection Section with Improved Evaporation Model. *Chemie-Ingenieur-Technik*, **2016**, 88, 1650-1664	0.8	8
76	On-line Analysis of Nitrogen Containing Compounds in Complex Hydrocarbon Matrixes. *Journal of Visualized Experiments*, **2016**,	1.6	4
75	Sophorolipid Amine Oxide Production by a Combination of Fermentation Scale-up and Chemical Modification. *Industrial & Engineering Chemistry Research*, **2016**, 55, 7273-7281	3.9	18
74	Potential of genetically engineered hybrid poplar for pyrolytic production of bio-based phenolic compounds. *Bioresource Technology*, **2016**, 207, 229-36	11	21
73	In situ performance of various metal doped catalysts in micro-pyrolysis and continuous fast pyrolysis. *Fuel Processing Technology*, **2016**, 144, 312-322	7.2	26
72	Evaluation of the transfection efficacies of quaternary ammonium salts prepared from sophorolipids. *Organic and Biomolecular Chemistry*, **2016**, 14, 3744-51	3.9	10
71	An experimental and kinetic modeling study of Δ-valerolactone pyrolysis. *Combustion and Flame*, **2016**, 164, 183-200	5.3	7
70	Chemical and enzymatic modification of sophorolipids. *Green Chemistry*, **2016**, 18, 76-104	10	39
69	Implementation of Stereochemistry in Automatic Kinetic Model Generation. *International Journal of Chemical Kinetics*, **2016**, 48, 755-769	1.4	3
68	Challenges and opportunities for molecule-based management of chemical processes. *Current Opinion in Chemical Engineering*, **2016**, 13, 142-149	5.4	15
67	Thermal Decomposition of Sulfur Compounds and their Role in Coke Formation during Steam Cracking of Heptane. *Chemical Engineering and Technology*, **2016**, 39, 2096-2106	2	6
66	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	5.3	16
65	Characterization and Comparison of Fast Pyrolysis Bio-oils from Pinewood, Rapeseed Cake, and Wheat Straw Using C NMR and Comprehensive GC ×GC. *ACS Sustainable Chemistry and Engineering*, **2016**, 4, 4974-4985	8.3	84
64	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, 556-569	1.4	1
63	Impact of flue gas radiative properties and burner geometry in furnace simulations. *AICHE Journal*, **2015**, 61, 936-954	3.6	20
62	JP-10 combustion studied with shock tube experiments and modeled with automatic reaction mechanism generation. *Combustion and Flame*, **2015**, 162, 3115-3129	5.3	57
61	Symmetry calculation for molecules and transition states. *Journal of Computational Chemistry*, **2015** , 36, 181-92	3.5	6
60	Rule-based ab initio kinetic model for alkyl sulfide pyrolysis. *Chemical Engineering Journal*, **2015**, 278, 385-393	14.7	22

59	A new class of antimicrobial biosurfactants: quaternary ammonium sophorolipids. *Green Chemistry*, **2015**, 17, 3373-3377	10	29
58	CFD-based design of 3D pyrolysis reactors: RANS vs. LES. *Chemical Engineering Journal*, **2015**, 282, 66-76	14.7	31
57	Catalytic Coating for Reduced Coke Formation in Steam Cracking Reactors. *Industrial & Engineering Chemistry Research*, **2015**, 54, 9525-9535	3.9	35
56	Pyrolysis and combustion chemistry of tetrahydropyran: Experimental and modeling study. *Combustion and Flame*, **2015**, 162, 4283-4303	5.3	17
55	Comprehensive compositional analysis of sulfur and nitrogen containing compounds in shale oil using GC □GC □FID/SCD/NCD/TOF-MS. *Fuel*, **2015**, 140, 398-406	7.1	83
54	Microkinetic model for the pyrolysis of methyl esters: From model compound to industrial biodiesel. *AICHE Journal*, **2015**, 61, 4309-4322	3.6	7
53	Necessity and Feasibility of 3D Simulations of Steam Cracking Reactors. *Industrial & Engineering Chemistry Research*, **2015**, 54, 12270-12282	3.9	21
52	Experimental and computational study of the initial decomposition of gamma-valerolactone. *Proceedings of the Combustion Institute*, **2015**, 35, 515-523	5.9	15
51	Kinetic Modeling of Jet Propellant-10 Pyrolysis. *Energy & Fuels*, **2015**, 29, 413-427	4.1	37
50	Impact of Radiation Models in Coupled Simulations of Steam Cracking Furnaces and Reactors. *Industrial & Engineering Chemistry Research*, **2015**, 54, 2453-2465	3.9	23
49	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, 199-231	1.4	80
48	Influence of the Reactor Material Composition on Coke Formation during Ethane Steam Cracking. *Industrial & Engineering Chemistry Research*, **2014**, 53, 6358-6371	3.9	43
47	Detailed compositional characterization of plastic waste pyrolysis oil by comprehensive two-dimensional gas-chromatography coupled to multiple detectors. *Journal of Chromatography A*, **2014**, 1359, 237-46	4.5	47
46	Coking Resistance of Specialized Coil Materials during Steam Cracking of Sulfur-Free Naphtha. *Industrial & Engineering Chemistry Research*, **2014**, 53, 13644-13655	3.9	29
45	Catalytic Fast Pyrolysis of Pine Wood: Effect of Successive Catalyst Regeneration. *Energy & Fuels*, **2014**, 28, 4560-4572	4.1	53
44	GPU based simulation of reactive mixtures with detailed chemistry in combination with tabulation and an analytical Jacobian. *Computers and Chemical Engineering*, **2014**, 71, 521-531	4	12
43	Combined Comprehensive Two-Dimensional Gas Chromatography Analysis of Polyaromatic Hydrocarbons/Polyaromatic Sulfur-Containing Hydrocarbons (PAH/PASH) in Complex Matrices. *Industrial & Engineering Chemistry Research*, **2014**, 53, 15436-15446	3.9	33
42	Experimental and Modeling Study on the Thermal Decomposition of Jet Propellant-10. *Energy & Fuels*, **2014**, 28, 4976-4985	4.1	36

41	Swirl flow tube reactor technology: An experimental and computational fluid dynamics study. *Chemical Engineering Journal*, **2014**, 238, 56-65	14.7	35
40	An experimental and kinetic modeling study of cyclopentadiene pyrolysis: First growth of polycyclic aromatic hydrocarbons. *Combustion and Flame*, **2014**, 161, 2739-2751	5.3	66
39	Computational fluid dynamics-based design of finned steam cracking reactors. *AICHE Journal*, **2014**, 60, 794-808	3.6	41
38	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, 18430-18442	3.9	15
37	Value Added Hydrocarbons from Distilled Tall Oil via Hydrotreating over a Commercial NiMo Catalyst. *Industrial & Engineering Chemistry Research*, **2013**, 52, 10114-10125	3.9	19
36	Production of bio-ethene and propene: alternatives for bulk chemicals and polymers. *Green Chemistry*, **2013**, 15, 3064	10	30
35	Validation of a new set-up for continuous catalytic fast pyrolysis of biomass coupled with vapour phase upgrading. *Journal of Analytical and Applied Pyrolysis*, **2013**, 103, 343-351	6	81
34	Laminar burning velocity of gasoline and the gasoline surrogate components iso-octane, n-heptane and toluene. *Fuel*, **2013**, 112, 355-365	7.1	170
33	The thermal decomposition of 2,5-dimethylfuran. *Proceedings of the Combustion Institute*, **2013**, 34, 251-258	3.9	66
32	Combustion and pyrolysis of iso-butanol: Experimental and chemical kinetic modeling study. *Combustion and Flame*, **2013**, 160, 1907-1929	5.3	61
31	Quantitative analysis of crude and stabilized bio-oils by comprehensive two-dimensional gas-chromatography. *Journal of Chromatography A*, **2012**, 1257, 131-40	4.5	109
30	Genesys: Kinetic model construction using chemo-informatics. *Chemical Engineering Journal*, **2012**, 207-208, 526-538	14.7	90
29	A comprehensive study of methyl decanoate pyrolysis. *Energy*, **2012**, 43, 146-160	7.9	33
28	Wood-derived olefins by steam cracking of hydrodeoxygenated tall oils. *Bioresource Technology*, **2012**, 126, 48-55	11	29
27	An Experimental and Kinetic Modeling Study of Pyrolysis and Combustion of AcetoneButanolEthanol (ABE) Mixtures. *Combustion Science and Technology*, **2012**, 184, 942-955	1.5	51
26	Coupled simulation of an industrial naphtha cracking furnace equipped with long-flame and radiation burners. *Computers and Chemical Engineering*, **2012**, 38, 24-34	4	25
25	Comprehensive CFD Simulation of Product Yields and Coking Rates for a Floor- and Wall-Fired Naphtha Cracking Furnace. *Industrial & Engineering Chemistry Research*, **2011**, 50, 13672-13685	3.9	27
24	Modeling the Composition of Crude Oil Fractions Using Constrained Homologous Series. *Industrial & Engineering Chemistry Research*, **2011**, 50, 10850-10858	3.9	24

23	Biomass to olefins: Cracking of renewable naphtha. *Chemical Engineering Journal*, **2011**, 176-177, 178-187	14.7	57
22	Comprehensive reaction mechanism for n-butanol pyrolysis and combustion. *Combustion and Flame* , **2011**, 158, 16-41	5.3	210
21	First principle-based simulation of ethane steam cracking. *AICHE Journal*, **2011**, 57, 482-496	3.6	51
20	Rapeseed oil methyl ester pyrolysis: on-line product analysis using comprehensive two-dimensional gas chromatography. *Journal of Chromatography A*, **2011**, 1218, 3217-23	4.5	47
19	Kinetic study of the thermal rearrangement of cis- and trans-2-pinanol. *Journal of Analytical and Applied Pyrolysis*, **2011**, 90, 187-196	6	9
18	Accurate High-Temperature Reaction Networks for Alternative Fuels: Butanol Isomers. *Industrial & Engineering Chemistry Research*, **2010**, 49, 10399-10420	3.9	68
17	Molecular reconstruction of complex hydrocarbon mixtures: An application of principal component analysis. *AICHE Journal*, **2010**, 56, 3174-3188	3.6	44
16	On-line analysis of complex hydrocarbon mixtures using comprehensive two-dimensional gas chromatography. *Journal of Chromatography A*, **2010**, 1217, 6623-33	4.5	78
15	Coke Formation in the Transfer Line Exchanger during Steam Cracking of Hydrocarbons. *Industrial & Engineering Chemistry Research*, **2009**, 48, 10343-10358	3.9	49
14	Influence of Silicon and Silicon/Sulfur-Containing Additives on Coke Formation during Steam Cracking of Hydrocarbons. *Industrial & Engineering Chemistry Research*, **2008**, 47, 1468-1482	3.9	40
13	Using elementary reactions to model growth processes of polyaromatic hydrocarbons under pyrolysis conditions of light feedstocks. *Molecular Simulation*, **2008**, 34, 193-199	2	11
12	Challenges of Modeling Steam Cracking of Heavy Feedstocks. *Oil and Gas Science and Technology*, **2008**, 63, 79-94	1.9	61
11	Evaluation of high-emissivity coatings in steam cracking furnaces using a non-grey gas radiation model. *Chemical Engineering Journal*, **2008**, 137, 411-421	14.7	42
10	Molecular reconstruction of naphtha steam cracking feedstocks based on commercial indices. *Computers and Chemical Engineering*, **2007**, 31, 1020-1034	4	70
9	Dimensional analysis for scaling up and down steam cracking coils. *Chemical Engineering Journal*, **2007**, 134, 3-10	14.7	43
8	Automatic reaction network generation using RMG for steam cracking of n-hexane. *AICHE Journal*, **2006**, 52, 718-730	3.6	97
7	Two Severity Indices for Scale-Up of Steam Cracking Coils. *Industrial & Engineering Chemistry Research*, **2005**, 44, 3402-3411	3.9	37
6	Effect of radial temperature profiles on yields in steam cracking. *AICHE Journal*, **2004**, 50, 173-183	3.6	57

5	Chemisorption of CO 2 in a gas–liquid vortex reactor: An interphase mass transfer efficiency assessment. *AICHE Journal*,	3.6	1
4	Toward an e-chemistree: Materials for electrification of the chemical industry. *MRS Bulletin*,1	3.2	3
3	Recent Advances in Pre-Treatment of Plastic Packaging Waste		2
2	The pyrolysis study of polybutadiene rubber under different structural and process parameters: comparison with polyvinyl chloride degradation. *Journal of Thermal Analysis and Calorimetry*,1	4.1	
1	Exceeding Equilibrium CO2 Conversion by Plasma-Assisted Chemical Looping. *ACS Energy Letters*,1896-1902	2021	0