Kevin Marcel Van Geem

List of Publications by Citations

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	Mechanical and chemical recycling of solid plastic waste. *Waste Management*, **2017**, 69, 24-58	8.6	858
237	New Trends in Olefin Production. *Engineering*, **2017**, 3, 171-178	9.7	320
236	Comprehensive reaction mechanism for n-butanol pyrolysis and combustion. *Combustion and Flame* , **2011**, 158, 16-41	5.3	210
235	Laminar burning velocity of gasoline and the gasoline surrogate components iso-octane, n-heptane and toluene. *Fuel*, **2013**, 112, 355-365	7.1	170
234	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
233	Automatic reaction network generation using RMG for steam cracking of n-hexane. *AICHE Journal*, **2006**, 52, 718-730	3.6	97
232	Genesys: Kinetic model construction using chemo-informatics. *Chemical Engineering Journal*, **2012**, 207-208, 526-538	14.7	90
231	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
230	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
229	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
228	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
227	On-line analysis of complex hydrocarbon mixtures using comprehensive two-dimensional gas chromatography. *Journal of Chromatography A*, **2010**, 1217, 6623-33	4.5	78
226	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
225	Molecular reconstruction of naphtha steam cracking feedstocks based on commercial indices. *Computers and Chemical Engineering*, **2007**, 31, 1020-1034	4	70
224	Accurate High-Temperature Reaction Networks for Alternative Fuels: Butanol Isomers. *Industrial & Engineering Chemistry Research*, **2010**, 49, 10399-10420	3.9	68
223	Towards closed-loop recycling of multilayer and coloured PET plastic waste by alkaline hydrolysis. *Green Chemistry*, **2020**, 22, 5376-5394	10	67
222	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

221	The thermal decomposition of 2,5-dimethylfuran. *Proceedings of the Combustion Institute*, **2013**, 34, 251-258	3.9	66
220	Upgrading the value of anaerobic digestion via chemical production from grid injected biomethane. *Energy and Environmental Science*, **2018**, 11, 1788-1802	35.4	64
219	Combustion and pyrolysis of iso-butanol: Experimental and chemical kinetic modeling study. *Combustion and Flame*, **2013**, 160, 1907-1929	5.3	61
218	Challenges of Modeling Steam Cracking of Heavy Feedstocks. *Oil and Gas Science and Technology*, **2008**, 63, 79-94	1.9	61
217	Challenges and opportunities of solvent-based additive extraction methods for plastic recycling. *Waste Management*, **2020**, 104, 148-182	8.6	60
216	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
215	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
214	Biomass to olefins: Cracking of renewable naphtha. *Chemical Engineering Journal*, **2011**, 176-177, 178-187	14.7	57
213	Effect of radial temperature profiles on yields in steam cracking. *AICHE Journal*, **2004**, 50, 173-183	3.6	57
212	Making chemicals with electricity. *Science*, **2019**, 364, 734-735	33.3	53
211	Catalytic Fast Pyrolysis of Pine Wood: Effect of Successive Catalyst Regeneration. *Energy & Fuels*, **2014**, 28, 4560-4572	4.1	53
210	Experimental and modeling study of the pyrolysis and combustion of dimethoxymethane. *Combustion and Flame*, **2018**, 190, 270-283	5.3	51
209	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
208	First principle-based simulation of ethane steam cracking. *AICHE Journal*, **2011**, 57, 482-496	3.6	51
207	Coke Formation in the Transfer Line Exchanger during Steam Cracking of Hydrocarbons. *Industrial & Engineering Chemistry Research*, **2009**, 48, 10343-10358	3.9	49
206	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
205	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
204	Molecular reconstruction of complex hydrocarbon mixtures: An application of principal component analysis. *AICHE Journal*, **2010**, 56, 3174-3188	3.6	44

203	Influence of the Reactor Material Composition on Coke Formation during Ethane Steam Cracking. *Industrial & Engineering Chemistry Research*, **2014**, 53, 6358-6371	3.9	43
202	Dimensional analysis for scaling up and down steam cracking coils. *Chemical Engineering Journal*, **2007**, 134, 3-10	14.7	43
201	A multi-layered view of chemical and biochemical engineering. *Chemical Engineering Research and Design*, **2020**, 155, A133-A145	5.5	43
200	Pressure dependent kinetic analysis of pathways to naphthalene from cyclopentadienyl recombination. *Combustion and Flame*, **2018**, 187, 247-256	5.3	42
199	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
198	Computational fluid dynamics-based design of finned steam cracking reactors. *AICHE Journal*, **2014**, 60, 794-808	3.6	41
197	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
196	Chemical and enzymatic modification of sophorolipids. *Green Chemistry*, **2016**, 18, 76-104	10	39
195	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
194	Kinetic Modeling of Jet Propellant-10 Pyrolysis. *Energy & Fuels*, **2015**, 29, 413-427	4.1	37
193	Two Severity Indices for Scale-Up of Steam Cracking Coils. *Industrial & Engineering Chemistry Research*, **2005**, 44, 3402-3411	3.9	37
192	Experimental and Modeling Study on the Thermal Decomposition of Jet Propellant-10. *Energy & Fuels*, **2014**, 28, 4976-4985	4.1	36
191	Catalytic Coating for Reduced Coke Formation in Steam Cracking Reactors. *Industrial & Engineering Chemistry Research*, **2015**, 54, 9525-9535	3.9	35
190	Swirl flow tube reactor technology: An experimental and computational fluid dynamics study. *Chemical Engineering Journal*, **2014**, 238, 56-65	14.7	35
189	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
188	A comprehensive study of methyl decanoate pyrolysis. *Energy*, **2012**, 43, 146-160	7.9	33
187	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
186	CFD-based design of 3D pyrolysis reactors: RANS vs. LES. *Chemical Engineering Journal*, **2015**, 282, 66-76	14.7	31

185	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
184	Production of bio-ethene and propene: alternatives for bulk chemicals and polymers. *Green Chemistry*, **2013**, 15, 3064	10	30
183	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
182	A new class of antimicrobial biosurfactants: quaternary ammonium sophorolipids. *Green Chemistry*, **2015**, 17, 3373-3377	10	29
181	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
180	Coking Resistance of Specialized Coil Materials during Steam Cracking of Sulfur-Free Naphtha. *Industrial & Engineering Chemistry Research*, **2014**, 53, 13644-13655	3.9	29
179	Wood-derived olefins by steam cracking of hydrodeoxygenated tall oils. *Bioresource Technology*, **2012**, 126, 48-55	11	29
178	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
177	Progress in Reaction Mechanisms and Reactor Technologies for Thermochemical Recycling of Poly(methyl methacrylate). *Polymers*, **2020**, 12,	4.5	27
176	Measuring biomass fast pyrolysis kinetics: State of the art. *Wiley Interdisciplinary Reviews: Energy and Environment*, **2019**, 8, e326	4.7	27
175	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
174	Artificial Intelligence in Steam Cracking Modeling: A Deep Learning Algorithm for Detailed Effluent Prediction. *Engineering*, **2019**, 5, 1027-1040	9.7	25
173	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
172	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
171	Modeling the Composition of Crude Oil Fractions Using Constrained Homologous Series. *Industrial & Engineering Chemistry Research*, **2011**, 50, 10850-10858	3.9	24
170	Sustainable innovations in steam cracking: CO2 neutral olefin production. *Reaction Chemistry and Engineering*, **2020**, 5, 239-257	4.9	24
169	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
168	A model of tetrahydrofuran low-temperature oxidation based on theoretically calculated rate constants. *Combustion and Flame*, **2018**, 191, 252-269	5.3	23

167	Quantitative compositional analysis of Estonian shale oil using comprehensive two dimensional gas chromatography. *Fuel Processing Technology*, **2017**, 167, 241-249	7.2	23
166	Impact of Radiation Models in Coupled Simulations of Steam Cracking Furnaces and Reactors. *Industrial & Engineering Chemistry Research*, **2015**, 54, 2453-2465	3.9	23
165	Optimization of the in Situ Pretreatment of High Temperature Ni□r Alloys for Ethane Steam Cracking. *Industrial & Engineering Chemistry Research*, **2017**, 56, 1424-1438	3.9	22
164	Rule-based ab initio kinetic model for alkyl sulfide pyrolysis. *Chemical Engineering Journal*, **2015**, 278, 385-393	14.7	22
163	Techno-economic assessment of mechanical recycling of challenging post-consumer plastic packaging waste. *Resources, Conservation and Recycling*, **2021**, 170, 105607	11.9	22
162	Experimental and modeling study of the pyrolysis and combustion of 2-methyl-tetrahydrofuran. *Combustion and Flame*, **2017**, 176, 409-428	5.3	21
161	Potential of genetically engineered hybrid poplar for pyrolytic production of bio-based phenolic compounds. *Bioresource Technology*, **2016**, 207, 229-36	11	21
160	Computational Fluid Dynamics-Assisted Process Intensification Study for Biomass Fast Pyrolysis in a Gas□olid Vortex Reactor. *Energy & Fuels*, **2018**, 32, 10169-10183	4.1	21
159	Necessity and Feasibility of 3D Simulations of Steam Cracking Reactors. *Industrial & Engineering Chemistry Research*, **2015**, 54, 12270-12282	3.9	21
158	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
157	Impact of flue gas radiative properties and burner geometry in furnace simulations. *AICHE Journal*, **2015**, 61, 936-954	3.6	20
156	Towards first-principles based kinetic modeling of biomass fast pyrolysis. *Biomass Conversion and Biorefinery*, **2017**, 7, 305-317	2.3	19
155	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
154	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
153	Pyrolysis and combustion chemistry of tetrahydropyran: Experimental and modeling study. *Combustion and Flame*, **2015**, 162, 4283-4303	5.3	17
152	Automated reaction database and reaction network analysis: extraction of reaction templates using cheminformatics. *Journal of Cheminformatics*, **2018**, 10, 11	8.6	17
151	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
150	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

149	Detailed Experimental and Kinetic Modeling Study of Cyclopentadiene Pyrolysis in the Presence of Ethene. *Energy & Fuels*, **2018**, 32, 3920-3934	4.1	15
148	Experimental and computational study of the initial decomposition of gamma-valerolactone. *Proceedings of the Combustion Institute*, **2015**, 35, 515-523	5.9	15
147	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
146	Challenges and opportunities for molecule-based management of chemical processes. *Current Opinion in Chemical Engineering*, **2016**, 13, 142-149	5.4	15
145	Machine Learning in Chemical Engineering: Strengths, Weaknesses, Opportunities, and Threats. *Engineering*, **2021**, 7, 1201-1201	9.7	15
144	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
143	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
142	Numerical and experimental evaluation of heat transfer in helically corrugated tubes. *AICHE Journal*, **2018**, 64, 1702-1713	3.6	14
141	Synthesis and Biological Evaluation of Bolaamphiphilic Sophorolipids. *ACS Sustainable Chemistry and Engineering*, **2018**, 6, 8992-9005	8.3	14
140	Quantitative on-line analysis of sulfur compounds in complex hydrocarbon matrices. *Journal of Chromatography A*, **2017**, 1509, 102-113	4.5	13
139	On-the-fly ab initio calculations toward accurate rate coefficients. *Proceedings of the Combustion Institute*, **2019**, 37, 283-290	5.9	13
138	Dynamic simulation of fouling in steam cracking reactors using CFD. *Chemical Engineering Journal*, **2017**, 329, 77-87	14.7	13
137	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
136	Decomposition and isomerization of 1-pentanol radicals and the pyrolysis of 1-pentanol. *Combustion and Flame*, **2018**, 196, 500-514	5.3	13
135	Periodic reactive flow simulation: Proof of concept for steam cracking coils. *AICHE Journal*, **2017**, 63, 1715-1726	3.6	12
134	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
133	The role of chemistry in the oscillating combustion of hydrocarbons: An experimental and theoretical study. *Chemical Engineering Journal*, **2020**, 385, 123401	14.7	12
132	Lipid-Based Quaternary Ammonium Sophorolipid Amphiphiles with Antimicrobial and Transfection Activities. *ChemSusChem*, **2019**, 12, 3642-3653	8.3	11

131	Using elementary reactions to model growth processes of polyaromatic hydrocarbons under pyrolysis conditions of light feedstocks. *Molecular Simulation*, **2008**, 34, 193-199	2	11
130	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
129	Microstructural Contributions of Different Polyolefins to the Deformation Mechanisms of Their Binary Blends. *Polymers*, **2020**, 12,	4.5	11
128	Group additive modeling of cyclopentane pyrolysis. *Journal of Analytical and Applied Pyrolysis*, **2017**, 128, 437-450	6	10
127	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
126	Compositional Characterization of Pyrolysis Fuel Oil from Naphtha and Vacuum Gas Oil. *Energy & Fuels*, **2018**, 32, 1276-1286	4.1	10
125	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
124	Evaluation of the transfection efficacies of quaternary ammonium salts prepared from sophorolipids. *Organic and Biomolecular Chemistry*, **2016**, 14, 3744-51	3.9	10
123	The thermal decomposition of furfural: molecular chemistry unraveled. *Proceedings of the Combustion Institute*, **2019**, 37, 445-452	5.9	10
122	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
121	Reuse of CO in energy intensive process industries. *Chemical Communications*, **2021**, 57, 10967-10982	5.8	10
120	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
119	Techno-economic analysis of an absorption based methanol to olefins recovery section. *Applied Thermal Engineering*, **2017**, 115, 477-490	5.8	9
118	Computational fluid dynamics-based steam cracking furnace optimization using feedstock flow distribution. *AICHE Journal*, **2017**, 63, 3199-3213	3.6	9
117	An experimental and numerical study of the suppression of jets, counterflow, and backflow in vortex units. *AICHE Journal*, **2019**, 65, e16614	3.6	9
116	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
115	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
114	Kinetic study of the thermal rearrangement of cis- and trans-2-pinanol. *Journal of Analytical and Applied Pyrolysis*, **2011**, 90, 187-196	6	9

113	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
112	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
111	Methane reforming to valuable products by an atmospheric pressure direct current discharge. *Journal of Cleaner Production*, **2019**, 209, 655-664	10.3	9
110	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
109	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
108	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
107	1D Model for Coupled Simulation of Steam Cracker Convection Section with Improved Evaporation Model. *Chemie-Ingenieur-Technik*, **2016**, 88, 1650-1664	0.8	8
106	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
105	Towards a Better Understanding of Delamination of Multilayer Flexible Packaging Films by Carboxylic Acids. *ChemSusChem*, **2021**, 14, 4198-4213	8.3	8
104	Effect of Long-Term High Temperature Oxidation on the Coking Behavior of Ni-Cr Superalloys. *Materials*, **2018**, 11,	3.5	8
103	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
102	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
101	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
100	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
99	Artificial Intelligence for Computer-Aided Synthesis In Flow: Analysis and Selection of Reaction Components. *Frontiers in Chemical Engineering*, **2020**, 2,	1	7
98	Ab initio derived group additivity model for intramolecular hydrogen abstraction reactions. *Physical Chemistry Chemical Physics*, **2018**, 20, 10877-10894	3.6	7
97	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
96	An experimental and kinetic modeling study of Δ-valerolactone pyrolysis. *Combustion and Flame*, **2016**, 164, 183-200	5.3	7

95	Microkinetic model for the pyrolysis of methyl esters: From model compound to industrial biodiesel. *AICHE Journal*, **2015**, 61, 4309-4322	3.6	7
94	Micromixing in a gas–liquid vortex reactor. *AICHE Journal*, **2021**, 67, e17264	3.6	7
93	catchyFOAM: Euler–Euler 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
92	Experimental and Kinetic Modeling Study of Cyclohexane Pyrolysis. *Energy & Fuels*, **2018**, 32, 7153-7168	4.2	7
91	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
90	Symmetry calculation for molecules and transition states. *Journal of Computational Chemistry*, **2015**, 36, 181-92	3.5	6
89	Experimental and kinetic modeling study of the pyrolysis and oxidation of diethylamine. *Fuel*, **2020**, 275, 117744	7.1	6
88	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
87	On the primary thermal decomposition pathways of hydroxycinnamic acids. *Proceedings of the Combustion Institute*, **2021**, 38, 4207-4214	5.9	6
86	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
85	An assessment of electrified methanol production from an environmental perspective. *Green Chemistry*, **2021**, 23, 7243-7258	10	6
84	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
83	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
82	Feasibility of biogas and oxy-fuel combustion in steam cracking furnaces: Experimental and computational study. *Fuel*, **2021**, 304, 121393	7.1	6
81	Hydrodynamic analysis of an axial impeller in a non-Newtonian fluid through particle image velocimetry. *AICHE Journal*, **2020**, 66, e16939	3.6	5
80	Evaluation of biological properties and fate in the environment of a new class of biosurfactants. *Chemosphere*, **2018**, 200, 561-568	8.4	5
79	CFD simulations of Industrial Steam Cracking Reactors: Turbulence–Chemistry Interaction and Dynamic Zoning. *Industrial & Engineering Chemistry Research*, **2017**, 56, 14959-14971	3.9	5
78	Pyrolysis of end-of-life polystyrene in a pilot-scale reactor: Maximizing styrene production.. *Waste Management*, **2021**, 139, 85-95	8.6	5

77	Deodorization of post-consumer plastic waste fractions: A comparison of different washing media.. *Science of the Total Environment*, **2021**, 812, 152467	10.2	5
76	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
75	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
74	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
73	Computational fluid dynamics-based optimization of dimpled steam cracking reactors for reduced CO2 emissions. *AICHE Journal*, **2020**, 66, e16255	3.6	4
72	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
71	On-line Analysis of Nitrogen Containing Compounds in Complex Hydrocarbon Matrixes. *Journal of Visualized Experiments*, **2016**,	1.6	4
70	Thermal Fouling of Heat Exchanger Tubes due to Heavy Hydrocarbon Droplets Impingement. *Heat Transfer Engineering*, **2017**, 38, 712-720	1.7	4
69	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
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