

Markus Kraft

List of Publications by Year in Descending Order

Source: <https://exaly.com/author-pdf/4451599/markus-kraft-publications-by-year.pdf>

Version: 2024-04-26

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

344
papers

10,369
citations

53
h-index

86
g-index

360
ext. papers

11,965
ext. citations

6.1
avg, IF

6.85
L-index

#	Paper	IF	Citations
344	Simulations of TiO ₂ nanoparticles synthesised off-centreline in jet-wall stagnation flames. <i>Journal of Aerosol Science</i> , 2022 , 162, 105928	4.3	0
343	Universal Digital Twin: Land use. <i>Data-Centric Engineering</i> , 2022 , 3,	2.6	2
342	Semantic 3D City Agents: An intelligent automation for dynamic geospatial knowledge graphs. <i>Energy and AI</i> , 2022 , 8, 100137	12.6	1
341	From Platform to Knowledge Graph: Evolution of Laboratory Automation.. <i>Jacs Au</i> , 2022 , 2, 292-309		6
340	Universal Digital Twin: The impact of heat pumps on social inequality. <i>Advances in Applied Energy</i> , 2022 , 5, 100079		2
339	ElChemo: A cross-domain interoperability between chemical and electrical systems in a plant. <i>Computers and Chemical Engineering</i> , 2022 , 156, 107556	4	3
338	Soot inception: Carbonaceous nanoparticle formation in flames. <i>Progress in Energy and Combustion Science</i> , 2022 , 88, 100956	33.6	17
337	On the reactive coagulation of incipient soot nanoparticles. <i>Journal of Aerosol Science</i> , 2022 , 159, 105866	4.3	2
336	Resource-optimised generation dispatch strategy for district heating systems using dynamic hierarchical optimisation. <i>Applied Energy</i> , 2022 , 305, 117877	10.7	0
335	The World Avatar: A World Model for Facilitating Interoperability. <i>Lecture Notes in Energy</i> , 2022 , 39-53	0.4	1
334	Cyber-Physical Systems in Decarbonisation. <i>Lecture Notes in Energy</i> , 2022 , 17-28	0.4	
333	Question answering system for chemistry: A semantic agent extension. <i>Digital Chemical Engineering</i> , 2022 , 3, 100032		0
332	Universal Digital Twin: Integration of national-scale energy systems and climate data. <i>Data-Centric Engineering</i> , 2022 , 3,	2.6	2
331	Understanding the particulate formation process in the engine fuelled with diesel/Jet A-1 blends. <i>Fuel</i> , 2021 , 313, 122675	7.1	1
330	How do the oxygenated functional groups in ether, carbonate and alcohol affect soot formation in Jet A2 diffusion flames?. <i>Combustion and Flame</i> , 2021 , 111849	5.3	1
329	Stochastic population balance methods for detailed modelling of flame-made aerosol particles. <i>Journal of Aerosol Science</i> , 2021 , 105895	4.3	1
328	Understanding the anatase-rutile stability in flame-made TiO ₂ . <i>Combustion and Flame</i> , 2021 , 226, 347-364	4.3	4

327	Automated Calibration of a Poly(oxyethylene) Dimethyl Ether Oxidation Mechanism Using the Knowledge Graph Technology. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 1701-1717	6.1	5
326	Game theory-based renewable multi-energy system design and subsidy strategy optimization. <i>Advances in Applied Energy</i> , 2021 , 2, 100024		14
325	Surface properties of heterogeneous polycyclic aromatic hydrocarbon clusters. <i>Proceedings of the Combustion Institute</i> , 2021 , 38, 1115-1123	5.9	2
324	On the thermophoretic sampling and TEM-based characterisation of soot particles in flames. <i>Carbon</i> , 2021 , 171, 711-722	10.4	12
323	Kinetic Monte Carlo statistics of curvature integration by HACA growth and bay closure reactions for PAH growth in a counterflow diffusion flame. <i>Proceedings of the Combustion Institute</i> , 2021 , 38, 1449-1457	5.9	4
322	Atomic insights into the sintering process of polycyclic aromatic hydrocarbon clusters. <i>Proceedings of the Combustion Institute</i> , 2021 , 38, 1181-1188	5.9	4
321	The effect of poly(oxyethylene) dimethyl ethers (PODE3) on soot formation in ethylene/PODE3 laminar coflow diffusion flames. <i>Fuel</i> , 2021 , 283, 118769	7.1	10
320	Aromatic penta-linked hydrocarbons in soot nanoparticle formation. <i>Proceedings of the Combustion Institute</i> , 2021 , 38, 1525-1532	5.9	7
319	Flame Synthesized Blue TiO with Tunable Oxygen Vacancies from Surface to Grain Boundary to Bulk.. <i>Small Methods</i> , 2021 , 5, e2000928	12.8	11
318	Mechanical Properties of Soot Particles: The Impact of Crosslinked Polycyclic Aromatic Hydrocarbons. <i>Combustion Science and Technology</i> , 2021 , 193, 643-663	1.5	9
317	Reactive localized Radicals on rim-based pentagonal rings: Properties and concentration in flames. <i>Proceedings of the Combustion Institute</i> , 2021 , 38, 565-573	5.9	6
316	Temperature and CH* measurements and simulations of laminar premixed ethylene jet-wall stagnation flames. <i>Proceedings of the Combustion Institute</i> , 2021 , 38, 2083-2091	5.9	0
315	Radical Aromatic Soot Precursors in Flames. <i>Journal of the American Chemical Society</i> , 2021 , 143, 12212-12219	12.6	10
314	Manipulating Intermediates at the Au/TiO ₂ Interface over InP Nanopillar Array for Photoelectrochemical CO ₂ Reduction. <i>ACS Catalysis</i> , 2021 , 11, 11416-11428	13.1	7
313	Question Answering System for Chemistry. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 3868-3880	3.8	3
312	The role of oxygenated species in the growth of graphene, fullerenes and carbonaceous particles. <i>Carbon</i> , 2021 , 182, 203-213	10.4	7
311	Predicting Power Conversion Efficiency of Organic Photovoltaics: Models and Data Analysis. <i>ACS Omega</i> , 2021 , 6, 23764-23775	3.9	5
310	How does a carbon tax affect Britain's power generation composition?. <i>Applied Energy</i> , 2021 , 298, 117117	10.7	4

309	Self-assembly of curved aromatic molecules in nanoparticles. <i>Carbon</i> , 2021 , 182, 70-88	10.4	1
308	Understanding the blending effect of polyoxymethylene dimethyl ethers as additive in a common-rail diesel engine. <i>Applied Energy</i> , 2021 , 300, 117380	10.7	5
307	Structural effects of C3 oxygenated fuels on soot formation in ethylene coflow diffusion flames. <i>Combustion and Flame</i> , 2021 , 232, 111512	5.3	4
306	Semantic 3D City Database [An enabler for a dynamic geospatial knowledge graph. <i>Energy and AI</i> , 2021 , 6, 100106	12.6	11
305	TiO ₂ with controllable oxygen vacancies for efficient isopropanol degradation: photoactivity and reaction mechanism. <i>Catalysis Science and Technology</i> , 2021 , 11, 4060-4071	5.5	4
304	Universal Digital Twin - A Dynamic Knowledge Graph. <i>Data-Centric Engineering</i> , 2021 , 2,	2.6	11
303	Wetting-regulated gas-involving (photo)electrocatalysis: biomimetics in energy conversion. <i>Chemical Society Reviews</i> , 2021 , 50, 10674-10699	58.5	10
302	Multiscale Cross-Domain Thermochemical Knowledge-Graph. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 6155-6166	6.1	9
301	OntoPowSys: A power system ontology for cross domain interactions in an eco industrial park. <i>Energy and AI</i> , 2020 , 1, 100008	12.6	20
300	J-Park Simulator: Wissensgraph für Industrie 4.0. <i>Chemie-Ingenieur-Technik</i> , 2020 , 92, 967-977	0.8	1
299	A density functional theory study on the kinetics of seven-member ring formation in polyaromatic hydrocarbons. <i>Combustion and Flame</i> , 2020 , 217, 152-174	5.3	5
298	The role of NO ₂ and NO in the mechanism of hydrocarbon degradation leading to carbonaceous deposits in engines. <i>Fuel</i> , 2020 , 267, 117218	7.1	4
297	Exploring the internal structure of soot particles using nanoindentation: A reactive molecular dynamics study. <i>Combustion and Flame</i> , 2020 , 219, 45-56	5.3	12
296	The impact of cyclic fuels on the formation and structure of soot. <i>Combustion and Flame</i> , 2020 , 219, 1-12	5.3	13
295	Study of industrial titania synthesis using a hybrid particle-number and detailed particle model. <i>Chemical Engineering Science</i> , 2020 , 219, 115615	4.4	6
294	Simulation of primary particle size distributions in a premixed ethylene stagnation flame. <i>Combustion and Flame</i> , 2020 , 216, 126-135	5.3	5
293	Linking reaction mechanisms and quantum chemistry: An ontological approach. <i>Computers and Chemical Engineering</i> , 2020 , 137, 106813	4	12
292	A Smart Contract-based agent marketplace for the J-Park Simulator - a knowledge graph for the process industry. <i>Computers and Chemical Engineering</i> , 2020 , 139, 106896	4	12

291	A virtual laboratory to support chemical reaction engineering courses using real-life problems and industrial software. <i>Education for Chemical Engineers</i> , 2020 , 33, 36-44	2.4	12
290	The impact of intelligent cyber-physical systems on the decarbonization of energy. <i>Energy and Environmental Science</i> , 2020 , 13, 744-771	35.4	39
289	Efficient simulation and auto-calibration of soot particle processes in Diesel engines. <i>Applied Energy</i> , 2020 , 262, 114484	10.7	5
288	Investigation of the impact of the configuration of exhaust after-treatment system for diesel engines. <i>Applied Energy</i> , 2020 , 267, 114844	10.7	22
287	A Parallel World Framework for scenario analysis in knowledge graphs. <i>Data-Centric Engineering</i> , 2020 , 1,	2.6	11
286	Rational Synthesis of Amorphous Iron-Nickel Phosphonates for Highly Efficient Photocatalytic Water Oxidation with Almost 100 % Yield. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 1171-1175	16.4	20
285	Rational Synthesis of Amorphous Iron-Nickel Phosphonates for Highly Efficient Photocatalytic Water Oxidation with Almost 100 % Yield. <i>Angewandte Chemie</i> , 2020 , 132, 1187-1191	3.6	4
284	OntoKin: An Ontology for Chemical Kinetic Reaction Mechanisms. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 108-120	6.1	27
283	On the coagulation efficiency of carbonaceous nanoparticles. <i>Journal of Aerosol Science</i> , 2020 , 140, 105478	4.9	16
282	Experimental study on engine combustion and particle size distributions fueled with Jet A-1. <i>Fuel</i> , 2020 , 263, 116747	7.1	13
281	A joint moment projection method and maximum entropy approach for simulation of soot formation and oxidation in diesel engines. <i>Applied Energy</i> , 2020 , 258, 114083	10.7	8
280	First Observation of an Acetate Switch in a Methanogenic Autotroph (S2). <i>Microbiology Insights</i> , 2020 , 13, 1178636120945300	2.5	0
279	Deep-Learning Architecture in QSPR Modeling for the Prediction of Energy Conversion Efficiency of Solar Cells. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 18991-19000	3.9	7
278	Reactivity of Polycyclic Aromatic Hydrocarbon Soot Precursors: Kinetics and Equilibria. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 10040-10052	2.8	11
277	Simultaneous design and operation optimization of renewable combined cooling heating and power systems. <i>AIChE Journal</i> , 2020 , 66, e17039	3.6	5
276	Deep kernel learning approach to engine emissions modeling. <i>Data-Centric Engineering</i> , 2020 , 1,	2.6	8
275	Knowledge Graph Approach to Combustion Chemistry and Interoperability. <i>ACS Omega</i> , 2020 , 5, 18342-18348	3.9	15
274	. <i>IEEE Transactions on Sustainable Energy</i> , 2020 , 11, 448-456	8.2	10

273	Evolution of the soot particle size distribution along the centreline of an n-heptane/toluene co-flow diffusion flame. <i>Combustion and Flame</i> , 2019 , 209, 256-266	5.3	17
272	From database to knowledge graph Using data in chemistry. <i>Current Opinion in Chemical Engineering</i> , 2019 , 26, 33-37	5.4	14
271	Topology of Disordered 3D Graphene Networks. <i>Physical Review Letters</i> , 2019 , 123, 116105	7.4	20
270	Reactivity of Polycyclic Aromatic Hydrocarbon Soot Precursors: Implications of Localized Radicals on Rim-Based Pentagonal Rings. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 26673-26682	3.8	30
269	Practically Useful Models for Kinetics of Biodiesel Production. <i>ACS Sustainable Chemistry and Engineering</i> , 2019 , 7, 4983-4992	8.3	3
268	Ion-Induced Soot Nucleation Using a New Potential for Curved Aromatics. <i>Combustion Science and Technology</i> , 2019 , 191, 747-765	1.5	13
267	Polymorphism of nanocrystalline TiO prepared in a stagnation flame: formation of the TiO-II phase. <i>Chemical Science</i> , 2019 , 10, 1342-1350	9.4	27
266	An assessment of the viability of alternatives to biodiesel transport fuels. <i>Applied Energy</i> , 2019 , 251, 113363	10.7	4
265	An Ontology and Semantic Web Service for Quantum Chemistry Calculations. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 3154-3165	6.1	20
264	Dynamic polarity of curved aromatic soot precursors. <i>Combustion and Flame</i> , 2019 , 206, 150-157	5.3	8
263	A two-step simulation methodology for modelling stagnation flame synthesised aggregate nanoparticles. <i>Combustion and Flame</i> , 2019 , 202, 143-153	5.3	14
262	Detailed characterisation of TiO ₂ nano-aggregate morphology using TEM image analysis. <i>Journal of Aerosol Science</i> , 2019 , 133, 96-112	4.3	10
261	Optimal site selection for modular nuclear power plants. <i>Computers and Chemical Engineering</i> , 2019 , 125, 339-350	4	21
260	Atomic structure and electronic structure of disordered graphitic carbon nitride. <i>Carbon</i> , 2019 , 147, 483-489	4.4	7
259	A hybrid particle-number and particle model for efficient solution of population balance equations. <i>Journal of Computational Physics</i> , 2019 , 389, 189-218	4.1	5
258	Nanostructure of Gasification Charcoal (Biochar). <i>Environmental Science & Technology</i> , 2019 , 53, 3538-3546	10.3	11
257	Analysing the effect of screw configuration using a stochastic twin-screw granulation model. <i>Chemical Engineering Science</i> , 2019 , 203, 358-379	4.4	4
256	Box-Behnken design based CO ₂ co-gasification of horticultural waste and sewage sludge with addition of ash from waste as catalyst. <i>Applied Energy</i> , 2019 , 242, 1549-1561	10.7	18

255	Modelling soot formation in a benchmark ethylene stagnation flame with a new detailed population balance model. <i>Combustion and Flame</i> , 2019 , 203, 56-71	5.3	27
254	Enhanced Procurement and Production Strategies for Chemical Plants: Utilizing Real-Time Financial Data and Advanced Algorithms. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 3072-3081	3.9	1
253	Polar curved polycyclic aromatic hydrocarbons in soot formation. <i>Proceedings of the Combustion Institute</i> , 2019 , 37, 1117-1123	5.9	27
252	Experimental and numerical study of the evolution of soot primary particles in a diffusion flame. <i>Proceedings of the Combustion Institute</i> , 2019 , 37, 2047-2055	5.9	21
251	Research advances towards large-scale solar hydrogen production from water. <i>EnergyChem</i> , 2019 , 1, 100014	36.9	82
250	A new methodology to calculate process rates in a kinetic Monte Carlo model of PAH growth. <i>Combustion and Flame</i> , 2019 , 209, 133-143	5.3	4
249	Sphere Encapsulated Monte Carlo: Obtaining Minimum Energy Configurations of Large Aromatic Systems. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 7303-7313	2.8	3
248	A detailed particle model for polydisperse aggregate particles. <i>Journal of Computational Physics</i> , 2019 , 397, 108799	4.1	14
247	Optical band gap of cross-linked, curved, and radical polyaromatic hydrocarbons. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 16240-16251	3.6	20
246	An agent composition framework for the J-Park Simulator - A knowledge graph for the process industry. <i>Computers and Chemical Engineering</i> , 2019 , 130, 106577	4	25
245	J-Park Simulator: An ontology-based platform for cross-domain scenarios in process industry. <i>Computers and Chemical Engineering</i> , 2019 , 131, 106586	4	27
244	Numerical simulation and parametric sensitivity study of titanium dioxide particles synthesised in a stagnation flame. <i>Journal of Aerosol Science</i> , 2019 , 138, 105451	4.3	11
243	Improved methodology for performing the inverse Abel transform of flame images for color ratio pyrometry. <i>Applied Optics</i> , 2019 , 58, 2662-2670	1.7	21
242	Modelling particle mass and particle number emissions during the active regeneration of diesel particulate filters. <i>Proceedings of the Combustion Institute</i> , 2019 , 37, 4831-4838	5.9	25
241	Partitioning of polycyclic aromatic hydrocarbons in heterogeneous clusters. <i>Carbon</i> , 2019 , 143, 247-256	10.4	14
240	Size spectra and source apportionment of fine particulates in tropical urban environment during southwest monsoon season. <i>Environmental Pollution</i> , 2019 , 244, 477-485	9.3	6
239	Extended first-principles thermochemistry for the oxidation of titanium tetrachloride. <i>Combustion and Flame</i> , 2019 , 199, 441-450	5.3	4
238	Bivariate extension of the moment projection method for the particle population balance dynamics. <i>Computers and Chemical Engineering</i> , 2019 , 124, 206-227	4	5

237	Internal structure of soot particles in a diffusion flame. <i>Carbon</i> , 2019 , 141, 635-642	10.4	50
236	Emerging applications of nanocatalysts synthesized by flame aerosol processes. <i>Current Opinion in Chemical Engineering</i> , 2018 , 20, 39-49	5.4	13
235	Co ₃ O ₄ and Fe _x Co _{3-x} O ₄ Nanoparticles/Films Synthesized in a Vapor-Fed Flame Aerosol Reactor for Oxygen Evolution. <i>ACS Applied Energy Materials</i> , 2018 , 1, 655-665	6.1	17
234	Sooting characteristics of polyoxymethylene dimethyl ether blends with diesel in a diffusion flame. <i>Fuel</i> , 2018 , 224, 499-506	7.1	38
233	Vapor Pressure and Heat of Vaporization of Molecules That Associate in the Gas Phase. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 5722-5731	3.9	3
232	A new iterative scheme for solving the discrete Smoluchowski equation. <i>Journal of Computational Physics</i> , 2018 , 352, 373-387	4.1	3
231	Incorporating seller/buyer reputation-based system in blockchain-enabled emission trading application. <i>Applied Energy</i> , 2018 , 209, 8-19	10.7	173
230	A systematic method to estimate and validate enthalpies of formation using error-cancelling balanced reactions. <i>Combustion and Flame</i> , 2018 , 187, 105-121	5.3	11
229	Evaluating smart sampling for constructing multidimensional surrogate models. <i>Computers and Chemical Engineering</i> , 2018 , 108, 276-288	4	10
228	Combustion modeling in RCCI engines with a hybrid characteristic time combustion and closed reactor model. <i>Applied Energy</i> , 2018 , 227, 665-671	10.7	3
227	A high-dimensional, stochastic model for twin-screw granulation [Part 1: Model description]. <i>Chemical Engineering Science</i> , 2018 , 188, 221-237	4.4	7
226	An adsorption-precipitation model for the formation of injector external deposits in internal combustion engines. <i>Applied Energy</i> , 2018 , 228, 1423-1438	10.7	13
225	Automated Advanced Calibration and Optimization of Thermochemical Models Applied to Biomass Gasification and Pyrolysis. <i>Energy & Fuels</i> , 2018 , 32, 10144-10153	4.1	6
224	An ontology framework towards decentralized information management for eco-industrial parks. <i>Computers and Chemical Engineering</i> , 2018 , 118, 49-63	4	30
223	An Ontology Based Cyber-infrastructure for the Development of Smart Eco Industrial Parks. <i>Computer Aided Chemical Engineering</i> , 2018 , 44, 2047-2052	0.6	0
222	A Highly Efficient Oxygen Evolution Catalyst Consisting of Interconnected Nickel-Iron-Layered Double Hydroxide and Carbon Nanodomains. <i>Advanced Materials</i> , 2018 , 30, 1705106	24	153
221	Smart adaptive sampling for developing surrogate approximations of physicochemical systems. <i>Computer Aided Chemical Engineering</i> , 2018 , 2191-2196	0.6	
220	Premixed Stagnation Flame Synthesized TiO ₂ Nanoparticles with Mixed Phases for Efficient Photocatalytic Hydrogen Generation. <i>ACS Sustainable Chemistry and Engineering</i> , 2018 , 6, 14470-14479	8.3	19

219	LEAPS2: Learning based Evolutionary Assistive Paradigm for Surrogate Selection. <i>Computers and Chemical Engineering</i> , 2018 , 119, 352-370	4	25
218	Flexoelectricity and the Formation of Carbon Nanoparticles in Flames. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 22210-22215	3.8	18
217	A high-dimensional, stochastic model for twin-screw granulation Part 2: Numerical methodology. <i>Chemical Engineering Science</i> , 2018 , 188, 18-33	4.4	4
216	Nickel Nanoparticles Encapsulated in Few-Layer Nitrogen-Doped Graphene Derived from Metal-Organic Frameworks as Efficient Bifunctional Electrocatalysts for Overall Water Splitting. <i>Advanced Materials</i> , 2017 , 29, 1605957	24	421
215	Theoretical Study of the Ti-Cl Bond Cleavage Reaction in TiCl ₄ . <i>Zeitschrift Fur Physikalische Chemie</i> , 2017 , 231, 1489-1506	3.1	3
214	A kinetic mechanism for the thermal decomposition of titanium tetraisopropoxide. <i>Proceedings of the Combustion Institute</i> , 2017 , 36, 1019-1027	5.9	22
213	A big data framework to validate thermodynamic data for chemical species. <i>Combustion and Flame</i> , 2017 , 176, 584-591	5.3	7
212	Screening and techno-economic assessment of biomass-based power generation with CCS technologies to meet 2050 CO ₂ targets. <i>Applied Energy</i> , 2017 , 190, 481-489	10.7	90
211	Development of a multi-compartment population balance model for high-shear wet granulation with discrete element method. <i>Computers and Chemical Engineering</i> , 2017 , 99, 171-184	4	21
210	Extension of moment projection method to the fragmentation process. <i>Journal of Computational Physics</i> , 2017 , 335, 516-534	4.1	23
209	Detailed population balance modelling of TiO ₂ synthesis in an industrial reactor. <i>Chemical Engineering Science</i> , 2017 , 164, 219-231	4.4	19
208	Modelling TiO ₂ formation in a stagnation flame using method of moments with interpolative closure. <i>Combustion and Flame</i> , 2017 , 178, 135-147	5.3	22
207	Outlier analysis for a silicon nanoparticle population balance model. <i>Combustion and Flame</i> , 2017 , 177, 89-97	5.3	3
206	Knowledge management of eco-industrial park for efficient energy utilization through ontology-based approach. <i>Applied Energy</i> , 2017 , 204, 1412-1421	10.7	32
205	Compartmental residence time estimation in batch granulators using a colourimetric image analysis algorithm and Discrete Element Modelling. <i>Advanced Powder Technology</i> , 2017 , 28, 2239-2255	4.6	8
204	Towards an ontological infrastructure for chemical process simulation and optimization in the context of eco-industrial parks. <i>Applied Energy</i> , 2017 , 204, 1284-1298	10.7	24
203	Efficient Combustion Modelling in RCCI Engine with Detailed Chemistry. <i>Energy Procedia</i> , 2017 , 105, 1582-1587	2.3	8
202	Design of computer experiments: A review. <i>Computers and Chemical Engineering</i> , 2017 , 106, 71-95	4	132

201	Blockchain technology in the chemical industry: Machine-to-machine electricity market. <i>Applied Energy</i> , 2017 , 195, 234-246	10.7	436
200	Self-template synthesis of CdS/NiS heterostructured nanohybrids for efficient photocatalytic hydrogen evolution. <i>Dalton Transactions</i> , 2017 , 46, 10650-10656	4.3	18
199	Developing breakage models relating morphological data to the milling behaviour of flame synthesised titania particles. <i>Chemical Engineering Science</i> , 2017 , 166, 53-65	4.4	8
198	The evolution of the biofuel science. <i>Renewable and Sustainable Energy Reviews</i> , 2017 , 76, 1479-1484	16.2	62
197	Unique P?Co?N Surface Bonding States Constructed on g-C3N4 Nanosheets for Drastically Enhanced Photocatalytic Activity of H2 Evolution. <i>Advanced Functional Materials</i> , 2017 , 27, 1604328	15.6	266
196	Modelling PAH curvature in laminar premixed flames using a detailed population balance model. <i>Combustion and Flame</i> , 2017 , 176, 172-180	5.3	24
195	Giant fullerene formation through thermal treatment of fullerene soot. <i>Carbon</i> , 2017 , 125, 132-138	10.4	26
194	Towards Intelligent Thermal Energy Management of Eco-industrial Park through Ontology-based Approach. <i>Energy Procedia</i> , 2017 , 105, 3295-3300	2.3	2
193	The Polarization of Polycyclic Aromatic Hydrocarbons Curved by Pentagon Incorporation: The Role of the Flexoelectric Dipole. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 27154-27163	3.8	40
192	Investigating the Role of Tunable Nitrogen Vacancies in Graphitic Carbon Nitride Nanosheets for Efficient Visible-Light-Driven H2 Evolution and CO2 Reduction. <i>ACS Sustainable Chemistry and Engineering</i> , 2017 , 5, 7260-7268	8.3	224
191	System Development for Eco-industrial Parks Using Ontological Innovation. <i>Energy Procedia</i> , 2017 , 105, 2239-2244	2.3	5
190	Smart Sampling Algorithm for Surrogate Model Development. <i>Computers and Chemical Engineering</i> , 2017 , 96, 103-114	4	41
189	A moment projection method for population balance dynamics with a shrinkage term. <i>Journal of Computational Physics</i> , 2017 , 330, 960-980	4.1	16
188	Soot particle size distributions in premixed stretch-stabilized flat ethyleneoxygenargon flames. <i>Proceedings of the Combustion Institute</i> , 2017 , 36, 1001-1009	5.9	30
187	Modelling of soot formation in a diesel engine with the moment projection method. <i>Energy Procedia</i> , 2017 , 142, 4092-4097	2.3	1
186	Modelling of secondary particulate emissions during the regeneration of Diesel Particulate Filters. <i>Energy Procedia</i> , 2017 , 142, 3560-3565	2.3	6
185	From Numerical Model to Computational Intelligence: The Digital Transition of Urban Energy System. <i>Energy Procedia</i> , 2017 , 143, 884-890	2.3	16
184	J-Park Simulator, an intelligent system for information management of eco-industrial parks. <i>Energy Procedia</i> , 2017 , 142, 2953-2958	2.3	7

183	Assessment of biodiesel plant waste heat recovery with respect to economics and CO ₂ emission. <i>Energy Procedia</i> , 2017 , 142, 1100-1105	2.3	1
182	J-park simulator 2017 ,		7
181	Numerical simulation and parametric sensitivity study of optical band gap in a laminar co-flow ethylene diffusion flame. <i>Combustion and Flame</i> , 2016 , 167, 320-334	5.3	22
180	Sooting tendency and particle size distributions of n-heptane/toluene mixtures burned in a wick-fed diffusion flame. <i>Fuel</i> , 2016 , 169, 111-119	7.1	49
179	Modelling soot formation from wall films in a gasoline direct injection engine using a detailed population balance model. <i>Applied Energy</i> , 2016 , 163, 154-166	10.7	68
178	PAH structure analysis of soot in a non-premixed flame using high-resolution transmission electron microscopy and optical band gap analysis. <i>Combustion and Flame</i> , 2016 , 164, 250-258	5.3	55
177	HRTEM evaluation of soot particles produced by the non-premixed combustion of liquid fuels. <i>Carbon</i> , 2016 , 96, 459-473	10.4	104
176	Smart Adaptive Sampling for Surrogate Modelling. <i>Computer Aided Chemical Engineering</i> , 2016 , 38, 631-636		3
175	Numerical and Experimental Study on Internal Nozzle Flow and Macroscopic Spray Characteristics of a Kind of Wide Distillation Fuel (WDF) - Kerosene 2016 ,		6
174	An Enhanced Primary Reference Fuel Mechanism Considering Conventional Fuel Chemistry in Engine Simulation. <i>Journal of Engineering for Gas Turbines and Power</i> , 2016 , 138,	1.7	6
173	Cambridge weblabs: A process control system using industrial standard SIMATIC PCS 7. <i>Education for Chemical Engineers</i> , 2016 , 16, 1-8	2.4	4
172	Design technologies for eco-industrial parks: From unit operations to processes, plants and industrial networks. <i>Applied Energy</i> , 2016 , 175, 305-323	10.7	49
171	Skeletal chemical mechanism of high-temperature TEOS oxidation in hydrogen/oxygen environment. <i>Combustion and Flame</i> , 2016 , 166, 243-254	5.3	10
170	Metal-free carbonaceous electrocatalysts and photocatalysts for water splitting. <i>Chemical Society Reviews</i> , 2016 , 45, 3039-52	58.5	419
169	Can nascent soot particles burn from the inside?. <i>Carbon</i> , 2016 , 109, 608-615	10.4	12
168	A novel methodology for the design of waste heat recovery network in eco-industrial park using techno-economic analysis and multi-objective optimization. <i>Applied Energy</i> , 2016 , 184, 88-102	10.7	34
167	Parameterisation of a biodiesel plant process flow sheet model. <i>Computers and Chemical Engineering</i> , 2016 , 95, 108-122	4	17
166	Microkinetic Modeling of the Fischer-Tropsch Synthesis over Cobalt Catalysts. <i>ChemCatChem</i> , 2015 , 7, 137-143	5.2	20

165	Numerical simulation and parametric sensitivity study of particle size distributions in a burner-stabilised stagnation flame. <i>Combustion and Flame</i> , 2015 , 162, 2569-2581	5.3	48
164	Quantitative tools for cultivating symbiosis in industrial parks; a literature review. <i>Applied Energy</i> , 2015 , 155, 599-612	10.7	71
163	First-Principles Thermochemistry for the Thermal Decomposition of Titanium Tetraisopropoxide. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 8376-87	2.8	28
162	Sooting tendency of surrogates for the aromatic fractions of diesel and gasoline in a wick-fed diffusion flame. <i>Fuel</i> , 2015 , 153, 31-39	7.1	46
161	Stochastic weighted particle methods for population balance equations with coagulation, fragmentation and spatial inhomogeneity. <i>Journal of Computational Physics</i> , 2015 , 303, 1-18	4.1	34
160	A detailed kinetic study of the thermal decomposition of tetraethoxysilane. <i>Proceedings of the Combustion Institute</i> , 2015 , 35, 2291-2298	5.9	22
159	Characterisation of lactose powder and granules for multivariate wet granulation modelling. <i>Chemical Engineering Science</i> , 2015 , 123, 395-405	4.4	11
158	Application of Dynamic ET Map: Analysis on a Natural Gas/Diesel Fueled RCCI Engine 2015 ,		1
157	Ab initio Variational Transition State Theory and Master Equation Study of the Reaction (OH)3SiOCH2 + CH3 ? (OH)3SiOC2H5. <i>Zeitschrift Fur Physikalische Chemie</i> , 2015 , 229, 691-708	3.1	5
156	Applying Industry 4.0 to the Jurong Island Eco-industrial Park. <i>Energy Procedia</i> , 2015 , 75, 1536-1541	2.3	68
155	Towards the Development of Carbon Dioxide Emission Landscape in Singapore. <i>Energy Procedia</i> , 2015 , 75, 2898-2903	2.3	2
154	Simulation and life cycle assessment of algae gasification process in dual fluidized bed gasifiers. <i>Green Chemistry</i> , 2015 , 17, 1793-1801	10	27
153	Impact of Urea Direct Injection on NOx Emission Formation of Diesel Engines Fueled by Biodiesel 2015 ,		1
152	Solid-liquid transitions in homogenous ovalene, hexabenzocoronene and circumcoronene clusters: A molecular dynamics study. <i>Combustion and Flame</i> , 2015 , 162, 486-495	5.3	30
151	Influence of experimental observations on n-propylbenzene kinetic parameter estimates. <i>Proceedings of the Combustion Institute</i> , 2015 , 35, 357-365	5.9	2
150	Surface reactivity of polycyclic aromatic hydrocarbon clusters. <i>Proceedings of the Combustion Institute</i> , 2015 , 35, 1811-1818	5.9	20
149	A multi-compartment population balance model for high shear granulation. <i>Computers and Chemical Engineering</i> , 2015 , 75, 1-13	4	10
148	The future viability of algae-derived biodiesel under economic and technical uncertainties. <i>Bioresour. Technol.</i> , 2014 , 151, 166-73	11	79

147	Size-dependent melting of polycyclic aromatic hydrocarbon nano-clusters: A molecular dynamics study. <i>Carbon</i> , 2014 , 67, 79-91	10.4	49
146	The carbon footprint and non-renewable energy demand of algae-derived biodiesel. <i>Applied Energy</i> , 2014 , 113, 1632-1644	10.7	67
145	Lifting a buried object: Reverse hopper theory. <i>Chemical Engineering Science</i> , 2014 , 105, 198-207	4.4	5
144	Stochastic solution of population balance equations for reactor networks. <i>Journal of Computational Physics</i> , 2014 , 256, 615-629	4.1	29
143	Phase change of polycyclic aromatic hydrocarbon clusters by mass addition. <i>Carbon</i> , 2014 , 77, 25-35	10.4	24
142	Production of Biorenewable Hydrogen and Syngas via Algae Gasification: A Sensitivity Analysis. <i>Energy Procedia</i> , 2014 , 61, 2767-2770	2.3	22
141	Particle Formation and Models 2014 , 1-23		22
140	Bayesian Error Propagation for a Kinetic Model of n-Propylbenzene Oxidation in a Shock Tube. <i>International Journal of Chemical Kinetics</i> , 2014 , 46, 389-404	1.4	26
139	Global sensitivity analysis of a model for silicon nanoparticle synthesis. <i>Journal of Aerosol Science</i> , 2014 , 76, 188-199	4.3	8
138	Sooting tendency of paraffin components of diesel and gasoline in diffusion flames. <i>Fuel</i> , 2014 , 126, 8-15	7.1	53
137	A new model for silicon nanoparticle synthesis. <i>Combustion and Flame</i> , 2013 , 160, 947-958	5.3	26
136	A fully coupled simulation of PAH and soot growth with a population balance model. <i>Proceedings of the Combustion Institute</i> , 2013 , 34, 1827-1835	5.9	71
135	Impact of powder characteristics on a particle granulation model. <i>Chemical Engineering Science</i> , 2013 , 97, 282-295	4.4	11
134	An improved methodology for determining threshold sooting indices from smoke point lamps. <i>Fuel</i> , 2013 , 111, 120-130	7.1	48
133	Bayesian parameter estimation for a jet-milling model using Metropolis Hastings and Wang-Landau sampling. <i>Chemical Engineering Science</i> , 2013 , 89, 244-257	4.4	21
132	Application of stochastic weighted algorithms to a multidimensional silica particle model. <i>Journal of Computational Physics</i> , 2013 , 248, 221-234	4.1	11
131	Techno-economic assessment of carbon-negative algal biodiesel for transport solutions. <i>Applied Energy</i> , 2013 , 106, 262-274	10.7	47
130	The Suitability of Particle Models in Capturing Aggregate Structure and Polydispersity. <i>Aerosol Science and Technology</i> , 2013 , 47, 734-745	3.4	15

129	Dual-Fuel Effects on HCCI Operating Range: Experiments with Primary Reference Fuels 2013 ,		2
128	Modelling Soot Formation: Model of Particle Formation. <i>Green Energy and Technology</i> , 2013 , 389-407	0.6	3
127	Spark ignition to homogeneous charge compression ignition mode transition study: a new modelling approach. <i>International Journal of Engine Research</i> , 2012 , 13, 540-564	2.7	1
126	A quantitative study of the clustering of polycyclic aromatic hydrocarbons at high temperatures. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 4081-94	3.6	117
125	A multidimensional population balance model to describe the aerosol synthesis of silica nanoparticles. <i>Journal of Aerosol Science</i> , 2012 , 44, 83-98	4.3	40
124	Synthesis of silicon nanoparticles with a narrow size distribution: A theoretical study. <i>Journal of Aerosol Science</i> , 2012 , 44, 46-61	4.3	18
123	The semantics of Chemical Markup Language (CML) for computational chemistry : CompChem. <i>Journal of Cheminformatics</i> , 2012 , 4, 15	8.6	18
122	HCCI Combustion Control Using Dual-Fuel Approach: Experimental and Modeling Investigations 2012 ,		11
121	Modelling the flame synthesis of silica nanoparticles from tetraethoxysilane. <i>Chemical Engineering Science</i> , 2012 , 70, 54-66	4.4	54
120	Iterative improvement of Bayesian parameter estimates for an engine model by means of experimental design. <i>Combustion and Flame</i> , 2012 , 159, 1303-1313	5.3	43
119	On a multivariate population balance model to describe the structure and composition of silica nanoparticles. <i>Computers and Chemical Engineering</i> , 2012 , 43, 130-147	4	31
118	Collaborative Sustainability Strategies for Online Laboratories 2012 , 468-490		0
117	Automated IC Engine Model Development with Uncertainty Propagation 2011 ,		9
116	Simulating PM Emissions and Combustion Stability in Gasoline/Diesel Fuelled Engines 2011 ,		16
115	Implementing Detailed Chemistry and In-Cylinder Stratification into 0/1-D IC Engine Cycle Simulation Tools 2011 ,		18
114	Optimisation of Injection Strategy, Combustion Characteristics and Emissions for IC Engines Using Advanced Simulation Technologies 2011 ,		9
113	Identifying Optimal Operating Points in Terms of Engineering Constraints and Regulated Emissions in Modern Diesel Engines 2011 ,		11
112	Multi-Objective Optimization of a Kinetics-Based HCCI Model Using Engine Data 2011 ,		5

111	Stochastic weighted particle methods for population balance equations. <i>Journal of Computational Physics</i> , 2011 , 230, 7456-7472	4.1	50
110	Theoretical insights into the surface growth of rutile TiO ₂ . <i>Combustion and Flame</i> , 2011 , 158, 1868-1876	5.3	20
109	A transferable electrostatic model for intermolecular interactions between polycyclic aromatic hydrocarbons. <i>Chemical Physics Letters</i> , 2011 , 510, 154-160	2.5	25
108	Modelling cycle to cycle variations in an SI engine with detailed chemical kinetics. <i>Combustion and Flame</i> , 2011 , 158, 179-188	5.3	21
107	Developing the PAH-PP soot particle model using process informatics and uncertainty propagation. <i>Proceedings of the Combustion Institute</i> , 2011 , 33, 675-683	5.9	88
106	The inverse problem in granulation modeling—two different statistical approaches. <i>AIChE Journal</i> , 2011 , 57, 3105-3121	3.6	25
105	A coupled CFD-population balance approach for nanoparticle synthesis in turbulent reacting flows. <i>Chemical Engineering Science</i> , 2011 , 66, 3792-3805	4.4	57
104	A survey of the potential energy surface for the (benzene) ₁₃ cluster. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 21362-6	3.6	10
103	Assessing the polycyclic aromatic hydrocarbon anisotropic potential with application to the exfoliation energy of graphite. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 13684-93	2.8	20
102	A mechanistic study on the simultaneous elimination of soot and nitric oxide from engine exhaust. <i>Carbon</i> , 2011 , 49, 1516-1531	10.4	47
101	First-principles thermochemistry for the combustion of TiCl ₄ in a methane flame. <i>Proceedings of the Combustion Institute</i> , 2011 , 33, 493-500	5.9	14
100	Modelling soot formation in a DISI engine. <i>Proceedings of the Combustion Institute</i> , 2011 , 33, 3159-3167	5.9	33
99	Simulating Combustion of Practical Fuels and Blends for Modern Engine Applications Using Detailed Chemical Kinetics 2010 ,		13
98	Experimental Investigation of a Control Method for SI-HCCI-SI Transition in a Multi-Cylinder Gasoline Engine. <i>SAE International Journal of Engines</i> , 2010 , 3, 928-937	2.4	14
97	A Fast Detailed-Chemistry Modelling Approach for Simulating the SI-HCCI Transition 2010 ,		3
96	Moving Toward Establishing More Robust and Systematic Model Development for IC Engines Using Process Informatics 2010 ,		6
95	Comment on "Low fractal dimension cluster-dilute soot aggregates from a premixed flame". <i>Physical Review Letters</i> , 2010 , 104, 119601; author reply 119602	7.4	13
94	A Detailed Chemistry Simulation of the SI-HCCI Transition. <i>SAE International Journal of Fuels and Lubricants</i> , 2010 , 3, 230-240	1.8	5

93	A First Principles Development of a General Anisotropic Potential for Polycyclic Aromatic Hydrocarbons. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 683-95	6.4	55
92	First-principles thermochemistry for gas phase species in an industrial rutile chlorinator. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 11825-32	2.8	7
91	Statistical Approximation of the Inverse Problem in Multivariate Population Balance Modeling. <i>Industrial & Engineering Chemistry Research</i> , 2010 , 49, 428-438	3.9	28
90	The future of computational modelling in reaction engineering. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2010 , 368, 3633-44	3	25
89	A Stochastic Algorithm for Parametric Sensitivity in Smoluchowski's Coagulation Equation. <i>SIAM Journal on Numerical Analysis</i> , 2010 , 48, 1064-1086	2.4	3
88	Coupling Algorithms for Calculating Sensitivities of Smoluchowski's Coagulation Equation. <i>SIAM Journal of Scientific Computing</i> , 2010 , 32, 635-655	2.6	7
87	2010 ,		15
86	Electronic and optical properties of aluminium-doped anatase and rutile TiO ₂ from ab initio calculations. <i>Physical Review B</i> , 2010 , 81,	3.3	115
85	Incorporating experimental uncertainties into multivariate granulation modelling. <i>Chemical Engineering Science</i> , 2010 , 65, 1088-1100	4.4	27
84	Numerical investigation of DQMoM-IEM as a turbulent reaction closure. <i>Chemical Engineering Science</i> , 2010 , 65, 1915-1924	4.4	38
83	Comparison of the stochastic fields method and DQMoM-IEM as turbulent reaction closures. <i>Chemical Engineering Science</i> , 2010 , 65, 5429-5441	4.4	22
82	Numerical study of a stochastic particle algorithm solving a multidimensional population balance model for high shear granulation. <i>Journal of Computational Physics</i> , 2010 , 229, 7672-7691	4.1	28
81	Parameter estimation in a multidimensional granulation model. <i>Powder Technology</i> , 2010 , 197, 196-210	5.2	56
80	Simulating the structural evolution of droplets following shell formation. <i>Chemical Engineering Science</i> , 2010 , 65, 713-725	4.4	63
79	Resolving conflicting parameter estimates in multivariate population balance models. <i>Chemical Engineering Science</i> , 2010 , 65, 4038-4045	4.4	12
78	A study on the coagulation of polycyclic aromatic hydrocarbon clusters to determine their collision efficiency. <i>Combustion and Flame</i> , 2010 , 157, 523-534	5.3	108
77	Modelling the internal structure of nascent soot particles. <i>Combustion and Flame</i> , 2010 , 157, 909-914	5.3	118
76	Mapping surrogate gasoline compositions into RON/MON space. <i>Combustion and Flame</i> , 2010 , 157, 1122-1131	5.1	192

75	New polycyclic aromatic hydrocarbon (PAH) surface processes to improve the model prediction of the composition of combustion-generated PAHs and soot. <i>Carbon</i> , 2010 , 48, 319-332	10.4	58
74	A Detailed Chemistry Multi-cycle Simulation of a Gasoline Fueled HCCI Engine Operated with NVO. <i>SAE International Journal of Fuels and Lubricants</i> , 2009 , 2, 13-27	1.8	17
73	Influence of Injection Timing and Piston Bowl Geometry on PCCI Combustion and Emissions. <i>SAE International Journal of Engines</i> , 2009 , 2, 1019-1033	2.4	40
72	HCCI Combustion Phasing Transient Control by Hydrogen-Rich Gas: Investigation Using a Fast Detailed-Chemistry Full-Cycle Model 2009 ,		11
71	A Detailed Model for the Sintering of Polydispersed Nanoparticle Agglomerates. <i>Aerosol Science and Technology</i> , 2009 , 43, 978-989	3.4	61
70	Modelling soot formation in a premixed flame using an aromatic-site soot model and an improved oxidation rate. <i>Proceedings of the Combustion Institute</i> , 2009 , 32, 639-646	5.9	94
69	A new model for the drying of droplets containing suspended solids. <i>Chemical Engineering Science</i> , 2009 , 64, 628-637	4.4	94
68	A new model for the drying of droplets containing suspended solids after shell formation. <i>Chemical Engineering Science</i> , 2009 , 64, 228-246	4.4	56
67	Towards a detailed soot model for internal combustion engines. <i>Combustion and Flame</i> , 2009 , 156, 1156-1165	11.65	128
66	A predictor-corrector algorithm for the coupling of stiff ODEs to a particle population balance. <i>Journal of Computational Physics</i> , 2009 , 228, 2758-2769	4.1	19
65	A statistical approach to develop a detailed soot growth model using PAH characteristics. <i>Combustion and Flame</i> , 2009 , 156, 896-913	5.3	104
64	A detailed kinetic model for combustion synthesis of titania from TiCl ₄ . <i>Combustion and Flame</i> , 2009 , 156, 1764-1770	5.3	45
63	The simultaneous reduction of nitric oxide and soot in emissions from diesel engines. <i>Carbon</i> , 2009 , 47, 866-875	10.4	54
62	First-principles thermochemistry for the combustion of a TiCl ₄ and AlCl ₃ mixture. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 13790-6	2.8	22
61	First-principles thermochemistry for silicon species in the decomposition of tetraethoxysilane. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 9041-9	2.8	34
60	Der Weg zu einem detaillierten Rußmodell für Verbrennungsmotoren. <i>MTZ - Motortechnische Zeitschrift</i> , 2009 , 70, 408-412	0.2	0
59	Towards a detailed soot model for internal combustion engines. <i>MTZ Worldwide</i> , 2009 , 70, 44-48	0.3	1
58	Towards a Detailed Soot Model for Internal Combustion Engines. <i>ATZ Autotechnology</i> , 2009 , 9, 54-57		

57	Modelling study of single walled carbon nanotube formation in a premixed flame. <i>Journal of Materials Chemistry</i> , 2008 , 18, 1582		13
56	Coupling Algorithms for Calculating Sensitivities of Population Balances 2008 ,		1
55	Real-Time Evaluation of a Detailed Chemistry HCCI Engine Model Using a Tabulation Technique. <i>Combustion Science and Technology</i> , 2008 , 180, 1263-1277	1.5	41
54	Studying the Influence of Direct Injection on PCCI Combustion and Emissions at Engine Idle Condition Using Two Dimensional CFD and Stochastic Reactor Model 2008 ,		14
53	Modes of neck growth in nanoparticle aggregates. <i>Combustion and Flame</i> , 2008 , 152, 272-275	5.3	9
52	Aromatic site description of soot particles. <i>Combustion and Flame</i> , 2008 , 155, 161-180	5.3	68
51	Modelling gas-phase synthesis of single-walled carbon nanotubes on iron catalyst particles. <i>Carbon</i> , 2008 , 46, 422-433	10.4	16
50	Toward a Comprehensive Model of the Synthesis of TiO ₂ Particles from TiCl ₄ . <i>Industrial & Engineering Chemistry Research</i> , 2007 , 46, 6147-6156	3.9	64
49	Two-stage Fuel Direct Injection in a Diesel Fuelled HCCI Engine 2007 ,		19
48	Formaldehyde and Hydroxyl Radicals in an HCCI Engine - Calculations and LIF-Measurements 2007 ,		9
47	Adsorption, diffusion and desorption of chlorine on and from rutile TiO ₂ {110}: a theoretical investigation. <i>ChemPhysChem</i> , 2007 , 8, 444-51	3.2	24
46	Models for the aggregate structure of soot particles. <i>Combustion and Flame</i> , 2007 , 151, 160-172	5.3	70
45	Modelling and validation of granulation with heterogeneous binder dispersion and chemical reaction. <i>Chemical Engineering Science</i> , 2007 , 62, 4717-4728	4.4	52
44	Numerical simulations of soot aggregation in premixed laminar flames. <i>Proceedings of the Combustion Institute</i> , 2007 , 31, 693-700	5.9	79
43	First-principles thermochemistry for the production of TiO ₂ from TiCl ₄ . <i>Journal of Physical Chemistry A</i> , 2007 , 111, 3560-5	2.8	62
42	Coupling a stochastic soot population balance to gas-phase chemistry using operator splitting. <i>Combustion and Flame</i> , 2007 , 148, 158-176	5.3	74
41	Dual injection homogeneous charge compression ignition engine simulation using a stochastic reactor model. <i>International Journal of Engine Research</i> , 2007 , 8, 41-50	2.7	47
40	Two methods for sensitivity analysis of coagulation processes in population balances by a Monte Carlo method. <i>Chemical Engineering Science</i> , 2006 , 61, 4966-4972	4.4	10

39	Extending stochastic soot simulation to higher pressures. <i>Combustion and Flame</i> , 2006 , 145, 638-642	5.3	59
38	A new numerical approach for the simulation of the growth of inorganic nanoparticles. <i>Journal of Computational Physics</i> , 2006 , 211, 638-658	4.1	58
37	Droplets population balance in a rotating disc contactor: An inverse problem approach. <i>AICHE Journal</i> , 2006 , 52, 1441-1450	3.6	32
36	An explicit numerical scheme for homogeneous gas-phase high-temperature combustion systems. <i>Combustion Theory and Modelling</i> , 2006 , 10, 171-182	1.5	4
35	The Linear Process Deferment Algorithm: A new technique for solving population balance equations. <i>SIAM Journal of Scientific Computing</i> , 2006 , 28, 303-320	2.6	63
34	Simulating a Homogeneous Charge Compression Ignition Engine Fuelled with a DEE/EtOH Blend 2006 ,		22
33	A new method for calculating the diameters of partially-sintered nanoparticles and its effect on simulated particle properties. <i>Chemical Engineering Science</i> , 2006 , 61, 158-166	4.4	13
32	Sources of CO emissions in an HCCI engine: A numerical analysis. <i>Combustion and Flame</i> , 2006 , 144, 634-637	5.3	39
31	Numerical simulation and sensitivity analysis of detailed soot particle size distribution in laminar premixed ethylene flames. <i>Combustion and Flame</i> , 2006 , 145, 117-127	5.3	124
30	A computational study of an HCCI engine with direct injection during gas exchange. <i>Combustion and Flame</i> , 2006 , 147, 118-132	5.3	40
29	Modelling nanoparticle dynamics: coagulation, sintering, particle inception and surface growth. <i>Combustion Theory and Modelling</i> , 2005 , 9, 449-461	1.5	25
28	A new algorithm for the direct simulation of combustion systems and its application to reaction elimination. <i>Proceedings of the Combustion Institute</i> , 2005 , 30, 1301-1308	5.9	5
27	Conservative method for the reduction of the number of particles in the Monte Carlo simulation method for kinetic equations. <i>Journal of Computational Physics</i> , 2005 , 203, 371-378	4.1	5
26	Single-particle method for stochastic simulation of coagulation processes. <i>Chemical Engineering Science</i> , 2005 , 60, 963-967	4.4	10
25	Stochastic modeling of soot particle size and age distributions in laminar premixed flames. <i>Proceedings of the Combustion Institute</i> , 2005 , 30, 1457-1465	5.9	75
24	NOx and N2O formation in HCCI engines 2005 ,		32
23	Evaluating the EGR-AFR Operating Range of a HCCI Engine 2005 ,		32
22	Direct Simulation and Mass Flow Stochastic Algorithms to Solve a Sintering-Coagulation Equation. <i>Monte Carlo Methods and Applications</i> , 2005 , 11,	0.4	15

21	Modelling a Dual-Fuelled Multi-Cylinder HCCI Engine Using a PDF Based Engine Cycle Simulator 2004,		24
20	A Monte Carlo methods for identification and sensitivity analysis of coagulation processes. <i>Journal of Computational Physics</i> , 2004 , 200, 50-59	4.1	26
19	Modelling of a RDC using a combined CFD-population balance approach. <i>Chemical Engineering Science</i> , 2004 , 59, 2597-2606	4.4	51
18	Simulation of coalescence and breakage: an assessment of two stochastic methods suitable for simulating liquid-liquid extraction. <i>Chemical Engineering Science</i> , 2004 , 59, 3865-3881	4.4	32
17	Partially Stirred Reactor Model: Analytical Solutions and Numerical Convergence Study of a PDF/Monte Carlo Method. <i>SIAM Journal of Scientific Computing</i> , 2004 , 25, 1798-1823	2.6	23
16	Homogeneous Charge Compression Ignition Engine: A Simulation Study on the Effects of Inhomogeneities. <i>Journal of Engineering for Gas Turbines and Power</i> , 2003 , 125, 466-471	1.7	37
15	Measurement and numerical simulation of soot particle size distribution functions in a laminar premixed ethylene-oxygen-argon flame. <i>Combustion and Flame</i> , 2003 , 133, 173-188	5.3	208
14	An improved stochastic algorithm for temperature-dependent homogeneous gas phase reactions. <i>Journal of Computational Physics</i> , 2003 , 185, 139-157	4.1	3
13	Numerical study of a stochastic particle method for homogeneous gas-phase reactions. <i>Computers and Mathematics With Applications</i> , 2003 , 45, 329-349	2.7	7
12	Analysis of the HCCI Combustion of a Turbocharged Truck Engine Using a Stochastic Reactor Model 2003,		9
11	An Efficient Stochastic Algorithm for Simulating Nano-particle Dynamics. <i>Journal of Computational Physics</i> , 2002 , 183, 210-232	4.1	79
10	Two approaches to the simulation of silica particle synthesis. <i>Proceedings of the Combustion Institute</i> , 2002 , 29, 1039-1046	5.9	12
9	Detailed modeling of soot formation in a partially stirred plug flow reactor. <i>Combustion and Flame</i> , 2002 , 128, 395-409	5.3	61
8	Analysis of the HCCI Combustion of a Turbocharged Truck Engine Using a Stochastic Reactor Model 2002, 97		4
7	Investigation of combustion emissions in a homogeneous charge compression injection engine: Measurements and a new computational model. <i>Proceedings of the Combustion Institute</i> , 2000 , 28, 1195-1201	5.9	93
6	Some analytic solutions for stochastic reactor models based on the joint composition PDF. <i>Combustion Theory and Modelling</i> , 1999 , 3, 343-358	1.5	4
5	PIC formation during the combustion of simple hydrocarbons in inhomogeneous incineration systems. <i>Proceedings of the Combustion Institute</i> , 1998 , 27, 1275-1281		4
4	Influence of turbulent mixing on the pyrolysis of chloroform using detailed chemical kinetics. <i>Proceedings of the Combustion Institute</i> , 1996 , 26, 2431-2437		4

3	Analysis of wet co oxidation under turbulent non-premixed conditions using a PDF method and detailed chemical kinetics. <i>Proceedings of the Combustion Institute</i> , 1996 , 26, 807-813	2
2	Semantic City Planning Systems (SCPS): A Literature Review. <i>Journal of Planning Literature</i> , 088541222110685	2
1	Modelling Investigation of the Thermal Treatment of Ash-Contaminated Particulate Filters. <i>Emission Control Science and Technology</i> , 1	2 0