S Mani Sarathy

List of Publications by Year in Descending Order

277 papers	9,768 citations	49 h-index	88 g-index
288 ext. papers	11,755 ext. citations	5.8 avg, IF	6.77 L-index

#	Paper	IF	Citations
277	Artificial intelligence□enabled fuel design **2022**, 47-67		
276	A decoupled modeling approach and experimental measurements for pyrolysis of C6-C10 saturated fatty acid methyl esters (FAMEs). *Combustion and Flame*, **2022**, 111955	5.3	2
275	A comprehensive neural network model for predicting flash point of oxygenated fuels using a functional group approach. *Fuel*, **2022**, 317, 123428	7.1	3
274	On the effects of CO2 atmosphere in the pyrolysis of Salicornia bigelovii. *Bioresource Technology Reports*, **2022**, 17, 100950	4.1	2
273	High purity, self-sustained, pressurized hydrogen production from ammonia in a catalytic membrane reactor. *Chemical Engineering Journal*, **2022**, 431, 134310	14.7	4
272	Ammonia and ammonia/hydrogen blends oxidation in a jet-stirred reactor: Experimental and numerical study. *Fuel*, **2022**, 310, 122202	7.1	2
271	On the lubricity mechanism of carbon-based nanofluid fuels. *Fuel*, **2022**, 308, 122031	7.1	
270	A reinforcement learning-based economic model predictive control framework for autonomous operation of chemical reactors. *Chemical Engineering Journal*, **2022**, 428, 130993	14.7	1
269	A Methodology for Designing Octane Number of Fuels Using Genetic Algorithms and Artificial Neural Networks. *Energy & Fuels*, **2022**, 36, 3867-3880	4.1	1
268	The effect of hydrogen bonding on the reactivity of OH radicals with prenol and isoprenol: a shock tube and multi-structural torsional variational transition state theory study.. *Physical Chemistry Chemical Physics*, **2022**,	3.6	3
267	Influence of gasoline fuel formulation on lean autoignition in a mixed-mode-combustion (deflagration/autoignition) engine. *Combustion and Flame*, **2022**, 242, 112163	5.3	0
266	Accurate thermochemistry prediction of extensive Polycyclic aromatic hydrocarbons (PAHs) and relevant radicals. *Combustion and Flame*, **2022**, 242, 112159	5.3	0
265	The impact of gasoline formulation on turbulent jet ignition. *Fuel*, **2022**, 324, 124373	7.1	2
264	Revisiting low temperature oxidation chemistry of n-heptane. *Combustion and Flame*, **2022**, 242, 112177	5.3	1
263	An experimental and kinetic modeling study of the pyrolysis of isoprene, a significant biogenic hydrocarbon in naturally occurring vegetation fires. *Combustion and Flame*, **2022**, 242, 112206	5.3	0
262	High-Temperature Pyrolysis and Combustion of C5□19 Fatty Acid Methyl Esters (FAMEs): A Lumped Kinetic Modeling Study. *Energy & Fuels*, **2021**, 35, 19553-19567	4.1	2
261	Evaporation, break-up, and pyrolysis of multi-component Arabian Light crude oil droplets at various temperatures. *International Journal of Heat and Mass Transfer*, **2021**, 183, 122175	4.9	3

260	Noncatalytic Oxidative Coupling of Methane (OCM): Gas-Phase Reactions in a Jet Stirred Reactor (JSR).. *ACS Omega*, **2021**, 6, 33757-33768	3.9	2
259	A techno-economic and life cycle assessment for the production of green methanol from CO2: catalyst and process bottlenecks. *Journal of Energy Chemistry*, **2021**, 68, 255-255	12	5
258	On the distillation of waste tire pyrolysis oil: A structural characterization of the derived fractions. *Fuel*, **2021**, 290, 120041	7.1	16
257	Early Chemistry of Nicotine Degradation in Heat-Not-Burn Smoking Devices and Conventional Cigarettes: Implications for Users and Second- and Third-Hand Smokers. *Journal of Physical Chemistry A*, **2021**, 125, 3177-3188	2.8	5
256	Pyrolysis of Waste Tires in a Twin-Auger Reactor Using CaO: Assessing the Physicochemical Properties of the Derived Products. *Energy & Fuels*, **2021**, 35, 8819-8833	4.1	4
255	Theoretical Study of an Undisclosed Reaction Class: Direct H-Atom Abstraction from Allylic Radicals by Molecular Oxygen. *Energies*, **2021**, 14, 2916	3.1	1
254	Predicting entropy and heat capacity of hydrocarbons using machine learning. *Energy and AI*, **2021**, 4, 100054	12.6	3
253	Polyether-Based Block Co(ter)polymers as Multifunctional Lubricant Additives. *ACS Applied Polymer Materials*, **2021**, 3, 3811-3820	4.3	4
252	Surrogate formulation and molecular characterization of sulfur species in vacuum residues using APPI and ESI FT-ICR mass spectrometry. *Fuel*, **2021**, 293, 120471	7.1	5
251	A functional-group-based approach to modeling real-fuel combustion chemistry II: Kinetic model construction and validation. *Combustion and Flame*, **2021**, 227, 510-525	5.3	6
250	A functional-group-based approach to modeling real-fuel combustion chemistry I: Prediction of stoichiometric parameters for lumped pyrolysis reactions. *Combustion and Flame*, **2021**, 227, 497-509	5.3	8
249	Chemical structure of atmospheric pressure premixed laminar formic acid/hydrogen flames. *Proceedings of the Combustion Institute*, **2021**, 38, 2379-2386	5.9	4
248	Three-stage auto-ignition of n-heptane and methyl-cyclohexane mixtures at lean conditions in a flat piston rapid compression machine. *Proceedings of the Combustion Institute*, **2021**, 38, 5539-5548	5.9	2
247	Understanding multi-stage HCCI combustion caused by thermal stratification and chemical three-stage auto-ignition. *Proceedings of the Combustion Institute*, **2021**, 38, 5575-5583	5.9	3
246	A comprehensive experimental and kinetic modeling study of 1- and 2-pentene. *Combustion and Flame*, **2021**, 223, 166-180	5.3	12
245	Simultaneous production of ketohydroperoxides from low temperature oxidation of a gasoline primary reference fuel mixture. *Fuel*, **2021**, 288, 119737	7.1	4
244	A theoretical study of the H- and HO2-assisted propen-2-ol tautomerizations: Reactive systems to evaluate collision efficiency definitions on chemically activated reactions using SS-QRRK theory. *Combustion and Flame*, **2021**, 225, 485-498	5.3	5
243	Experimental and theoretical evidence for the temperature-determined evolution of PAH functional groups. *Proceedings of the Combustion Institute*, **2021**, 38, 1467-1475	5.9	5

242	Using deep neural networks to diagnose engine pre-ignition. *Proceedings of the Combustion Institute*, **2021**, 38, 5915-5922	5.9	1
241	A technological roadmap to the ammonia energy economy: Current state and missing technologies. *Chemical Engineering Journal*, **2021**, 408, 127310	14.7	28
240	A lumped kinetic model for high-temperature pyrolysis and combustion of 50 surrogate fuel components and their mixtures. *Fuel*, **2021**, 286, 119361	7.1	10
239	Counterflow ignition and extinction of FACE gasoline fuels. *Proceedings of the Combustion Institute*, **2021**, 38, 2323-2331	5.9	1
238	Understanding the synergistic blending octane behavior of 2-methylfuran. *Proceedings of the Combustion Institute*, **2021**, 38, 5625-5633	5.9	2
237	Probing the Chemical Kinetics of Minimalist Functional Group Gasoline Surrogates. *Energy & Fuels*, **2021**, 35, 3315-3332	4.1	8
236	Polymeric waste valorization at a crossroads: ten ways to bridge the research on model and complex/real feedstock. *Green Chemistry*, **2021**, 23, 4656-4664	10	1
235	Efficient alkane oxidation under combustion engine and atmospheric conditions. *Communications Chemistry*, **2021**, 4,	6.3	11
234	One-step conversion of crude oil to light olefins using a multi-zone reactor. *Nature Catalysis*, **2021**, 4, 233-241	36.5	21
233	The Role of Intermediate-Temperature Heat Release in Octane Sensitivity of Fuels with Matching Research Octane Number. *Energy & Fuels*, **2021**, 35, 4457-4477	4.1	4
232	Rapid soot inception via alkynyl substitution of polycyclic aromatic hydrocarbons. *Fuel*, **2021**, 295, 120580	7.1	13
231	Atomistic simulations of syngas oxy-combustion in supercritical CO2. *Journal of CO2 Utilization*, **2021**, 49, 101554	7.6	1
230	Effects of ammonia addition on soot formation in ethylene laminar premixed flames. *Combustion and Flame*, **2021**, 111698	5.3	2
229	Hydrogen Evolution from Hydrocarbon Pyrolysis in a Simulated Liquid Metal Bubble Reactor. *Energy & Fuels*, **2021**, 35, 14597-14609	4.1	1
228	Unraveling the octane response of gasoline/ethanol blends: Paving the way to formulating gasoline surrogates. *Fuel*, **2021**, 299, 120882	7.1	7
227	Probing the gas-phase oxidation of ammonia: Addressing uncertainties with theoretical calculations. *Combustion and Flame*, **2021**, 111708	5.3	1
226	An investigation into the pyrolysis and oxidation of bio-oil from sugarcane bagasse: Kinetics and evolved gases using TGA-FTIR. *Journal of Environmental Chemical Engineering*, **2021**, 9, 106144	6.8	7
225	On the origins of lubricity and surface cleanliness in ethanol-diesel fuel blends. *Fuel*, **2021**, 302, 121135	7.1	2

224	A comprehensive combustion chemistry study of n-propylcyclohexane. *Combustion and Flame*, **2021**, 233, 111576	5.3	4
223	Combustion chemistry of ammonia/hydrogen mixtures: Jet-stirred reactor measurements and comprehensive kinetic modeling. *Combustion and Flame*, **2021**, 234, 111653	5.3	14
222	Low-temperature oxidation chemistry of 2,4,4-trimethyl-1-pentene (diisobutylene) triggered by dimethyl ether (DME): A jet-stirred reactor oxidation and kinetic modeling investigation. *Combustion and Flame*, **2021**, 234, 111629	5.3	0
221	Bio-oil and biochar production from halophyte biomass: effects of pre-treatment and temperature on Salicornia bigelovii pyrolysis. *Sustainable Energy and Fuels*, **2021**, 5, 2234-2248	5.8	5
220	Laminar Burning Velocities of Formic Acid and Formic Acid/Hydrogen Flames: An Experimental and Modeling Study. *Energy & Fuels*, **2021**, 35, 1760-1767	4.1	2
219	Gas-to-Liquid Phase Transition of PAH at Flame Temperatures. *Journal of Physical Chemistry A*, **2020**, 124, 3896-3903	2.8	6
218	Identification of volatile constituents released from IQOS heat-not-burn tobacco HeatSticks using a direct sampling method. *Tobacco Control*, **2020**,	5.3	4
217	Understanding the blending octane behaviour of unsaturated hydrocarbons: A case study of C4 molecules and comparison with toluene. *Fuel*, **2020**, 275, 117971	7.1	2
216	Screening gas-phase chemical kinetic models: Collision limit compliance and ultrafast timescales. *International Journal of Chemical Kinetics*, **2020**, 52, 599-610	1.4	6
215	Laminar Burning Velocities and Kinetic Modeling of a Renewable E-Fuel: Formic Acid and Its Mixtures with H2 and CO2. *Energy & Fuels*, **2020**, 34, 7564-7572	4.1	13
214	A Systematic Theoretical Kinetics Analysis for the Waddington Mechanism in the Low-Temperature Oxidation of Butene and Butanol Isomers. *Journal of Physical Chemistry A*, **2020**, 124, 5646-5656	2.8	6
213	Oxidation kinetics of n-pentanol: A theoretical study of the reactivity of the 1-hydroxy-1-peroxypentyl radical. *Combustion and Flame*, **2020**, 219, 20-32	5.3	11
212	Investigating the Effects of C3 and C4 Alcohol Blending on Ignition Quality of Gasoline Fuels. *Energy & Fuels*, **2020**, 34, 8777-8787	4.1	0
211	Kinetics of the benzyl + HO and benzoxyl + OH barrierless association reactions: fate of the benzyl hydroperoxide adduct under combustion and atmospheric conditions. *Physical Chemistry Chemical Physics*, **2020**, 22, 9029-9039	3.6	0
210	PAH formation from jet stirred reactor pyrolysis of gasoline surrogates. *Combustion and Flame*, **2020**, 219, 312-326	5.3	21
209	Autoignition of diethyl ether and a diethyl ether/ethanol blend. *Fuel*, **2020**, 279, 118553	7.1	9
208	Enhanced lubrication by core-shell TiO2 nanoparticles modified with gallic acid ester. *Tribology International*, **2020**, 146, 106263	4.9	12
207	Spray combustion simulation study of waste cooking oil biodiesel and diesel under direct injection diesel engine conditions. *Fuel*, **2020**, 267, 117240	7.1	14

206	Chemical kinetics of hydroxyl reactions with cyclopentadiene and indene. *Combustion and Flame*, **2020**, 217, 48-56	5.3	6
205	CO2 Derived E-Fuels: Research Trends, Misconceptions, and Future Directions. *Trends in Chemistry*, **2020**, 2, 785-795	14.8	15
204	Analyzing the solid soot particulates formed in a fuel-rich flame by solvent-free matrix-assisted laser desorption/ionization Fourier transform ion cyclotron resonance mass spectrometry. *Rapid Communications in Mass Spectrometry*, **2020**, 34, e8596	2.2	5
203	Developing a Theoretical Approach for Accurate Determination of the Density and Thermochemical Properties of Energetic Ionic Liquids. *Propellants, Explosives, Pyrotechnics*, **2020**, 45, 1949-1958	1.7	1
202	Cool flame chemistry of diesel surrogate compounds: n-Decane, 2-methylnonane, 2,7-dimethyloctane, and n-butylcyclohexane. *Combustion and Flame*, **2020**, 219, 384-392	5.3	5
201	Global sensitivity analysis of n-butanol ignition delay times to thermodynamics class and rate rule parameters. *Combustion and Flame*, **2020**, 222, 355-369	5.3	5
200	Probing hydrogen□itrogen chemistry: A theoretical study of important reactions in NxHy, HCN and HNCO oxidation. *International Journal of Hydrogen Energy*, **2020**, 45, 23624-23637	6.7	9
199	Data Science Approach to Estimate Enthalpy of Formation of Cyclic Hydrocarbons. *Journal of Physical Chemistry A*, **2020**, 124, 6270-6276	2.8	7
198	Chemical and kinetic insights into fuel lubricity loss of low-sulfur diesel upon the addition of multiple oxygenated compounds. *Tribology International*, **2020**, 152, 106559	4.9	7
197	Investigating Water Injection in Single-Cylinder Gasoline Spark-Ignited Engines at Fixed Speed. *Energy & Fuels*, **2020**, 34, 16636-16653	4.1	3
196	Exploring low temperature oxidation of 1-butene in jet-stirred reactors. *Combustion and Flame*, **2020**, 222, 259-271	5.3	5
195	Effects of fuel composition variability on high temperature combustion properties: A statistical analysis. *Applications in Energy and Combustion Science*, **2020**, 1-4, 100012	0.8	0
194	Techno-Economic Analysis of Pressurized Oxy-Fuel Combustion of Petroleum Coke. *Energies*, **2020**, 13, 3463	3.1	8
193	Multi-stage heat release in lean combustion: Insights from coupled tangential stretching rate (TSR) and computational singular perturbation (CSP) analysis. *Combustion and Flame*, **2020**, 219, 242-257	5.3	5
192	Collision Efficiency Parameter Influence on Pressure-Dependent Rate Constant Calculations Using the SS-QRRK Theory. *Journal of Physical Chemistry A*, **2020**, 124, 6277-6286	2.8	5
191	Ignition delay time measurements of diesel and gasoline blends. *Combustion and Flame*, **2020**, 222, 460-475	5.3	5
190	A droplet reactor on a super-hydrophobic surface allows control and characterization of amyloid fibril growth. *Communications Biology*, **2020**, 3, 457	6.7	6
189	Fuel and Chemical Properties of Waste Tire Pyrolysis Oil Derived from a Continuous Twin-Auger Reactor. *Energy & Fuels*, **2020**, 34, 12688-12702	4.1	20

188	Impact of OH Radical Generator Involvement in the Gas-Phase Radical Reaction Network on the Oxidative Coupling of Methane: A Simulation Study. *Energy Technology*, **2020**, 8, 1900563	3.5	7
187	Bridging the gap in a resource and climate-constrained world with advanced gasoline compression-ignition hybrids. *Applied Energy*, **2020**, 267, 114936	10.7	18
186	Machine Learning To Predict Standard Enthalpy of Formation of Hydrocarbons. *Journal of Physical Chemistry A*, **2019**, 123, 8305-8313	2.8	22
185	Exploring the combustion chemistry of a novel lignocellulose-derived biofuel: cyclopentanol. Part I: quantum chemistry calculation and kinetic modeling. *Combustion and Flame*, **2019**, 210, 490-501	5.3	12
184	Chemical Ignition Characteristics of Ethanol Blending with Primary Reference Fuels. *Energy & Fuels*, **2019**, 33, 10185-10196	4.1	20
183	Chemical kinetic study of triptane (2,2,3-trimethylbutane) as an anti-knock additive. *Combustion and Flame*, **2019**, 210, 399-412	5.3	1
182	The influence of chemical composition on ignition delay times of gasoline fractions. *Combustion and Flame*, **2019**, 209, 418-429	5.3	16
181	Ethanolic gasoline, a lignocellulosic advanced biofuel. *Sustainable Energy and Fuels*, **2019**, 3, 409-421	5.8	8
180	Ion chemistry in premixed rich methane flames. *Combustion and Flame*, **2019**, 202, 208-218	5.3	16
179	Characterization of deasphalted heavy fuel oil using APPI (+) FT-ICR mass spectrometry and NMR spectroscopy. *Fuel*, **2019**, 253, 950-963	7.1	29
178	Autoignition Characteristics of Ethers Blended with Low Cetane Distillates. *Energy & Fuels*, **2019**, 33, 6775-6787	4.1	8
177	Experimental and numerical investigations on the laminar burning velocity of n-butanol + air mixtures at elevated temperatures. *Fuel*, **2019**, 249, 36-44	7.1	8
176	Development of a reduced four-component (toluene/n-heptane/iso-octane/ethanol) gasoline surrogate model. *Fuel*, **2019**, 247, 164-178	7.1	33
175	On the opposing effects of methanol and ethanol addition on PAH and soot formation in ethylene counterflow diffusion flames. *Combustion and Flame*, **2019**, 202, 228-242	5.3	55
174	Computational study of polycyclic aromatic hydrocarbons growth by vinylacetylene addition. *Combustion and Flame*, **2019**, 202, 276-291	5.3	31
173	Methylcyclohexane pyrolysis and oxidation in a jet-stirred reactor. *Proceedings of the Combustion Institute*, **2019**, 37, 409-417	5.9	22
172	Polycyclic aromatic hydrocarbons in pyrolysis of gasoline surrogates (n-heptane/iso-octane/toluene). *Proceedings of the Combustion Institute*, **2019**, 37, 993-1001	5.9	33
171	Small ester combustion chemistry: Computational kinetics and experimental study of methyl acetate and ethyl acetate. *Proceedings of the Combustion Institute*, **2019**, 37, 419-428	5.9	27

170	Evolution of oxygenated polycyclic aromatic hydrocarbon chemistry at flame temperatures. *Combustion and Flame*, **2019**, 209, 441-451	5.3	21
169	Environmental Challenges and Opportunities in Marine Engine Heavy Fuel Oil Combustion. *Lecture Notes in Civil Engineering*, **2019**, 1047-1055	0.3	6
168	Computational singular perturbation analysis of brain lactate metabolism. *PLoS ONE*, **2019**, 14, e0226094	3.7	7
167	Oxidative-Coupling-Assisted Methane Aromatization: A Simulation Study. *Industrial & Engineering Chemistry Research*, **2019**, 58, 22884-22892	3.9	4
166	Auto-ignition of direct injection spray of light naphtha, primary reference fuels, gasoline and gasoline surrogate. *Energy*, **2019**, 170, 375-390	7.9	15
165	Three-stage heat release in n-heptane auto-ignition. *Proceedings of the Combustion Institute*, **2019**, 37, 485-492	5.9	31
164	Low temperature autoignition of 5-membered ring naphthenes: Effects of substitution. *Combustion and Flame*, **2019**, 200, 387-404	5.3	21
163	The site effect on PAHs formation in HACA-based mass growth process. *Combustion and Flame*, **2019**, 199, 54-68	5.3	48
162	Surrogate formulation for diesel and jet fuels using the minimalist functional group (MFG) approach. *Proceedings of the Combustion Institute*, **2019**, 37, 4663-4671	5.9	28
161	Exploring gasoline oxidation chemistry in jet stirred reactors. *Fuel*, **2019**, 236, 1282-1292	7.1	29
160	Measurement of laminar burning velocity of n-pentanol + air mixtures at elevated temperatures and a skeletal kinetic model. *Fuel*, **2019**, 237, 10-17	7.1	15
159	A comparative study on the sooting tendencies of various 1-alkene fuels in counterflow diffusion flames. *Combustion and Flame*, **2018**, 192, 71-85	5.3	27
158	High-Pressure Limit Rate Rules for □H Isomerization of Hydroperoxyalkylperoxy Radicals. *Journal of Physical Chemistry A*, **2018**, 122, 3626-3639	2.8	14
157	Impact of thermodynamic properties and heat loss on ignition of transportation fuels in rapid compression machines. *Fuel*, **2018**, 218, 203-212	7.1	3
156	Predicting Octane Number Using Nuclear Magnetic Resonance Spectroscopy and Artificial Neural Networks. *Energy & Fuels*, **2018**, 32, 6309-6329	4.1	68
155	2-Methylfuran: A bio-derived octane booster for spark-ignition engines. *Fuel*, **2018**, 225, 349-357	7.1	20
154	A minimalist functional group (MFG) approach for surrogate fuel formulation. *Combustion and Flame*, **2018**, 192, 250-271	5.3	47
153	Cool diffusion flames of butane isomers activated by ozone in the counterflow. *Combustion and Flame*, **2018**, 191, 175-186	5.3	16

152	Ab initio and transition state theory study of the OH + HO -rHO + O()/O() reactions: yield and role of O() in HO decomposition and in combustion of H. *Physical Chemistry Chemical Physics*, **2018**, 20, 4478-4489	3.6	18
151	Theoretical kinetic study of the formic acid catalyzed Criegee intermediate isomerization: multistructural anharmonicity and atmospheric implications. *Physical Chemistry Chemical Physics*, **2018**, 20, 10806-10814	3.6	19
150	CH4/air homogeneous autoignition: A comparison of two chemical kinetics mechanisms. *Fuel*, **2018**, 223, 74-85	7.1	19
149	A surrogate fuel formulation to characterize heating and evaporation of light naphtha droplets. *Combustion Science and Technology*, **2018**, 190, 1218-1231	1.5	9
148	Theoretical Kinetic Study of the Unimolecular Keto-Enol Tautomerism Propen-2-ol <-rAcetone. Pressure Effects and Implications in the Pyrolysis of tert- and 2-Butanol. *Journal of Physical Chemistry A*, **2018**, 122, 3547-3555	2.8	15
147	Chemical kinetic insights into the ignition dynamics of n-hexane. *Combustion and Flame*, **2018**, 188, 28-40	5.3	32
146	n-Heptane cool flame chemistry: Unraveling intermediate species measured in a stirred reactor and motored engine. *Combustion and Flame*, **2018**, 187, 199-216	5.3	47
145	Chemical Kinetic Modeling Study on the Influence of n-Butanol Blending on the Combustion, Autoignition, and Knock Properties of Gasoline and Its Surrogate in a Spark-Ignition Engine. *Energy & Fuels*, **2018**, 32, 10065-10077	4.1	3
144	Lube Products: Molecular Characterization of Base Oils **2018**, 1-14		5
143	Global sensitivity analysis of n-butanol reaction kinetics using rate rules. *Combustion and Flame*, **2018**, 196, 452-465	5.3	13
142	Computational Kinetics of Hydroperoxybutylperoxy Isomerizations and Decompositions: A Study of the Effect of Hydrogen Bonding. *Journal of Physical Chemistry A*, **2018**, 122, 6277-6291	2.8	6
141	Extensive Theoretical Study of the Thermochemical Properties of Unsaturated Hydrocarbons and Allylic and Super-Allylic Radicals: The Development and Optimization of Group Additivity Values. *Journal of Physical Chemistry A*, **2018**, 122, 4736-4749	2.8	21
140	Autoignition of straight-run naphtha: A promising fuel for advanced compression ignition engines. *Combustion and Flame*, **2018**, 189, 337-346	5.3	20
139	Numerical investigation of injector geometry effects on fuel stratification in a GCI engine. *Fuel*, **2018**, 214, 580-589	7.1	35
138	Recent progress in gasoline surrogate fuels. *Progress in Energy and Combustion Science*, **2018**, 65, 67-108	33.6	215
137	Estimating fuel octane numbers from homogeneous gas-phase ignition delay times. *Combustion and Flame*, **2018**, 188, 307-323	5.3	28
136	Ab Initio, Transition State Theory, and Kinetic Modeling Study of the HO-Assisted Keto-Enol Tautomerism Propen-2-ol + HO <-Acetone + HO under Combustion, Atmospheric, and Interstellar Conditions. *Journal of Physical Chemistry A*, **2018**, 122, 9792-9805	2.8	12
135	Effectiveness of Fuel Enrichment on Knock Suppression in a Gasoline Spark-Ignited Engine **2018**,		9

134	Effect of Mixture Formation and Injection Strategies on Stochastic Pre-Ignition **2018**,		14
133	Reduced Gasoline Surrogate (Toluene/n-Heptane/iso-Octane) Chemical Kinetic Model for Compression Ignition Simulations **2018**,		10
132	The Influence of Intake Pressure and Ethanol Addition to Gasoline on Single- and Dual-Stage Autoignition in an HCCI Engine. *Energy & Fuels*, **2018**, 32, 9822-9837	4.1	5
131	An experimental and chemical kinetic modeling study of 1,3-butadiene combustion: Ignition delay time and laminar flame speed measurements. *Combustion and Flame*, **2018**, 197, 423-438	5.3	240
130	Automated chemical kinetic mechanism simplification with minimal user expertise. *Combustion and Flame*, **2018**, 197, 439-448	5.3	13
129	Analysis of the current–voltage curves and saturation currents in burner-stabilised premixed flames with detailed ion chemistry and transport models. *Combustion Theory and Modelling*, **2018**, 22, 939-972	1.5	8
128	Ignition delay time sensitivity in ignition quality tester (IQT) and its relation to octane sensitivity. *Fuel*, **2018**, 233, 412-419	7.1	15
127	Oxidation of 2-methylfuran and 2-methylfuran/n-heptane blends: An experimental and modeling study. *Combustion and Flame*, **2018**, 196, 54-70	5.3	25
126	New insights into methane-oxygen ion chemistry. *Proceedings of the Combustion Institute*, **2017**, 36, 1213-1221	5.9	22
125	Variations in non-thermal NO formation pathways in alcohol flames. *Proceedings of the Combustion Institute*, **2017**, 36, 3995-4002	5.9	11
124	Impact of fuel molecular structure on auto-ignition behavior – Design rules for future high performance gasolines. *Progress in Energy and Combustion Science*, **2017**, 60, 1-25	33.6	117
123	Premixed flame chemistry of a gasoline primary reference fuel surrogate. *Combustion and Flame*, **2017**, 179, 300-311	5.3	11
122	Chemical Kinetic Insights into the Octane Number and Octane Sensitivity of Gasoline Surrogate Mixtures. *Energy & Fuels*, **2017**, 31, 1945-1960	4.1	77
121	A comprehensive iso-octane combustion model with improved thermochemistry and chemical kinetics. *Combustion and Flame*, **2017**, 178, 111-134	5.3	130
120	Compositional effects on PAH and soot formation in counterflow diffusion flames of gasoline surrogate fuels. *Combustion and Flame*, **2017**, 178, 46-60	5.3	69
119	An extensive experimental and modeling study of 1-butene oxidation. *Combustion and Flame*, **2017**, 181, 198-213	5.3	57
118	Cyclopentane combustion. Part II. Ignition delay measurements and mechanism validation. *Combustion and Flame*, **2017**, 183, 372-385	5.3	36
117	High temperature shock tube experiments and kinetic modeling study of diisopropyl ketone ignition and pyrolysis. *Combustion and Flame*, **2017**, 177, 207-218	5.3	20

116	Quantities of Interest in Jet Stirred Reactor Oxidation of a High-Octane Gasoline. *Energy & Fuels*, **2017**, 31, 5543-5553	4.1	16
115	Achieving 80% greenhouse gas reduction target in Saudi Arabia under low and medium oil prices. *Energy Policy*, **2017**, 101, 502-511	7.2	11
114	Heavy fuel oil pyrolysis and combustion: Kinetics and evolved gases investigated by TGA-FTIR. *Journal of Analytical and Applied Pyrolysis*, **2017**, 127, 183-195	6	48
113	Theoretical Kinetics Analysis for H Atom Addition to 1,3-Butadiene and Related Reactions on the H Potential Energy Surface. *Journal of Physical Chemistry A*, **2017**, 121, 7433-7445	2.8	34
112	Optimizing Blendstock Composition and Ethanol Feedstock to Reduce Gasoline Well-to-Pump CO 2 Emission. *Energy Procedia*, **2017**, 105, 3642-3647	2.3	1
111	Optimization of the octane response of gasoline/ethanol blends. *Applied Energy*, **2017**, 203, 778-793	10.7	51
110	On the effects of fuel properties and injection timing in partially premixed compression ignition of low octane fuels. *Fuel*, **2017**, 207, 373-388	7.1	32
109	Ignition studies of two low-octane gasolines. *Combustion and Flame*, **2017**, 185, 152-159	5.3	43
108	Autoignition characteristics of oxygenated gasolines. *Combustion and Flame*, **2017**, 186, 114-128	5.3	50
107	Unraveling the structure and chemical mechanisms of highly oxygenated intermediates in oxidation of organic compounds. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 13102-13107	11.5	80
106	Heats of Formation of Medium-Sized Organic Compounds from Contemporary Electronic Structure Methods. *Journal of Chemical Theory and Computation*, **2017**, 13, 3537-3560	6.4	29
105	Integrated In Situ Characterization of a Molten Salt Catalyst Surface: Evidence of Sodium Peroxide and Hydroxyl Radical Formation. *Angewandte Chemie*, **2017**, 129, 10539-10543	3.6	11
104	Integrated In Situ Characterization of a Molten Salt Catalyst Surface: Evidence of Sodium Peroxide and Hydroxyl Radical Formation. *Angewandte Chemie - International Edition*, **2017**, 56, 10403-10407	16.4	36
103	Cyclopentane combustion chemistry. Part I: Mechanism development and computational kinetics. *Combustion and Flame*, **2017**, 183, 358-371	5.3	38
102	Performance and emissions of gasoline blended with terpineol as an octane booster. *Renewable Energy*, **2017**, 101, 1087-1093	8.1	26
101	Ignition characteristics of 2-methyltetrahydrofuran: An experimental and kinetic study. *Proceedings of the Combustion Institute*, **2017**, 36, 587-595	5.9	24
100	Aromatic ring formation in opposed-flow diffusive 1,3-butadiene flames. *Proceedings of the Combustion Institute*, **2017**, 36, 947-955	5.9	30
99	Understanding premixed flame chemistry of gasoline fuels by comparing quantities of interest. *Proceedings of the Combustion Institute*, **2017**, 36, 1203-1211	5.9	12

98	Antiknock quality and ignition kinetics of 2-phenylethanol, a novel lignocellulosic octane booster. *Proceedings of the Combustion Institute*, **2017**, 36, 3515-3522	5.9	15
97	New insights into the low-temperature oxidation of 2-methylhexane. *Proceedings of the Combustion Institute*, **2017**, 36, 373-382	5.9	30
96	The influence of n -butanol blending on the ignition delay times of gasoline and its surrogate at high pressures. *Fuel*, **2017**, 187, 211-219	7.1	25
95	Measurements of Positively Charged Ions in Premixed Methane-Oxygen Atmospheric Flames. *Combustion Science and Technology*, **2017**, 189, 575-594	1.5	10
94	Jet-stirred reactor oxidation of alkane-rich FACE gasoline fuels. *Proceedings of the Combustion Institute*, **2017**, 36, 517-524	5.9	23
93	The oxidation of 2-butene: A high pressure ignition delay, kinetic modeling study and reactivity comparison with isobutene and 1-butene. *Proceedings of the Combustion Institute*, **2017**, 36, 403-411	5.9	268
92	A laminar flame investigation of 2-butanone, and the combustion-related intermediates formed through its oxidation. *Proceedings of the Combustion Institute*, **2017**, 36, 1175-1183	5.9	17
91	Elucidating reactivity regimes in cyclopentane oxidation: Jet stirred reactor experiments, computational chemistry, and kinetic modeling. *Proceedings of the Combustion Institute*, **2017**, 36, 469-477	5.9	27
90	Ignition delay measurements of light naphtha: A fully blended low octane fuel. *Proceedings of the Combustion Institute*, **2017**, 36, 315-322	5.9	44
89	Terpineol as a novel octane booster for extending the knock limit of gasoline. *Fuel*, **2017**, 187, 9-15	7.1	24
88	Blending Behavior of Ethanol with PRF 84 and FACE A Gasoline in HCCI Combustion Mmode **2017**,		8
87	Simulating HCCI Blending Octane Number of Primary Reference Fuel with Ethanol **2017**,		17
86	Improved combustion kinetic model and HCCI engine simulations of di-isopropyl ketone ignition. *Fuel*, **2016**, 164, 141-150	7.1	20
85	Lifecycle optimized ethanol-gasoline blends for turbocharged engines. *Applied Energy*, **2016**, 181, 38-53	10.7	35
84	Predicting Fuel Ignition Quality Using 1H NMR Spectroscopy and Multiple Linear Regression. *Energy & Fuels*, **2016**, 30, 9819-9835	4.1	60
83	Experimental and Chemical Kinetic Modeling Study of Dimethylcyclohexane Oxidation and Pyrolysis. *Energy & Fuels*, **2016**, 30, 8648-8657	4.1	9
82	Effects of Substitution on Counterflow Ignition and Extinction of C3 and C4 Alcohols. *Energy & Fuels*, **2016**, 30, 6091-6097	4.1	14
81	Effects of methyl substitution on the auto-ignition of C16 alkanes. *Combustion and Flame*, **2016**, 164, 259-269	5.3	27

80	A blending rule for octane numbers of PRFs and TPRFs with ethanol. *Fuel*, **2016**, 180, 175-186	7.1	54
79	A computational study of ethylene□air sooting flames: Effects of large polycyclic aromatic hydrocarbons. *Combustion and Flame*, **2016**, 163, 427-436	5.3	39
78	A comprehensive experimental and modeling study of isobutene oxidation. *Combustion and Flame*, **2016**, 167, 353-379	5.3	220
77	Modeling Ignition of a Heptane Isomer: Improved Thermodynamics, Reaction Pathways, Kinetics, and Rate Rule Optimizations for 2-Methylhexane. *Journal of Physical Chemistry A*, **2016**, 120, 2201-17	2.8	43
76	Additional chain-branching pathways in the low-temperature oxidation of branched alkanes. *Combustion and Flame*, **2016**, 164, 386-396	5.3	72
75	Compositional Effects of Gasoline Fuels on Combustion, Performance and Emissions in Engine. *SAE International Journal of Fuels and Lubricants*, **2016**, 9, 460-468	1.8	13
74	Blending Octane Number of Ethanol in HCCI, SI and CI Combustion Modes. *SAE International Journal of Fuels and Lubricants*, **2016**, 9, 659-682	1.8	37
73	□Pinene - A High Energy Density Biofuel for SI Engine Applications **2016**,		8
72	Experimental and Numerical Investigation of Ethanol/Diethyl Ether Mixtures in a CI Engine **2016**,		13
71	Mixing-structure relationship in jet-stirred reactors. *Chemical Engineering Research and Design*, **2016** , 111, 461-464	5.5	15
70	Third O2 addition reactions promote the low-temperature auto-ignition of n-alkanes. *Combustion and Flame*, **2016**, 165, 364-372	5.3	55
69	Calculation of Average Molecular Parameters, Functional Groups, and a Surrogate Molecule for Heavy Fuel Oils Using 1H and 13C Nuclear Magnetic Resonance Spectroscopy. *Energy & Fuels*, **2016**, 30, 3894-3905	4.1	55
68	Compositional effects on the ignition of FACE gasolines. *Combustion and Flame*, **2016**, 169, 171-193	5.3	139
67	Fuel Class Higher Alcohols **2016**, 29-57		5
66	Two-stage Lagrangian modeling of ignition processes in ignition quality tester and constant volume combustion chambers. *Fuel*, **2016**, 185, 589-598	7.1	12
65	Optimized reaction mechanism rate rules for ignition of normal alkanes. *Combustion and Flame*, **2016**, 173, 468-482	5.3	96
64	An experimental and modeling study of diethyl carbonate oxidation. *Combustion and Flame*, **2015**, 162, 1395-1405	5.3	20
63	Shock tube and modeling study of 2,7-dimethyloctane pyrolysis and oxidation. *Combustion and Flame*, **2015**, 162, 2296-2306	5.3	14

62	Analysis of impact of temperature and saltwater on Nannochloropsis salina bio-oil production by ultra high resolution APCI FT-ICR MS. *Algal Research*, **2015**, 9, 227-235	5	20
61	A comprehensive experimental and modeling study of 2-methylbutanol combustion. *Combustion and Flame*, **2015**, 162, 2166-2176	5.3	28
60	Kinetics of ethylcyclohexane pyrolysis and oxidation: An experimental and detailed kinetic modeling study. *Combustion and Flame*, **2015**, 162, 2873-2892	5.3	47
59	Experiments and simulations of NOx formation in the combustion of hydroxylated fuels. *Combustion and Flame*, **2015**, 162, 2322-2336	5.3	13
58	Structural Level Characterization of Base Oils Using Advanced Analytical Techniques. *Energy & Fuels*, **2015**, 29, 2962-2970	4.1	41
57	Effect of the Methyl Substitution on the Combustion of Two Methylheptane Isomers: Flame Chemistry Using Vacuum-Ultraviolet (VUV) Photoionization Mass Spectrometry. *Energy & Fuels* , **2015**, 29, 2696-2708	4.1	7
56	Numerical modelling of ion transport in flames. *Combustion Theory and Modelling*, **2015**, 19, 744-772	1.5	16
55	Combustion Characteristics of C5 Alcohols and a Skeletal Mechanism for Homogeneous Charge Compression Ignition Combustion Simulation. *Energy & Fuels*, **2015**, 29, 7584-7594	4.1	18
54	Mixed butanols addition to gasoline surrogates: Shock tube ignition delay time measurements and chemical kinetic modeling. *Combustion and Flame*, **2015**, 162, 3971-3979	5.3	30
53	A methodology to relate octane numbers of binary and ternary n-heptane, iso-octane and toluene mixtures with simulated ignition delay times. *Fuel*, **2015**, 160, 458-469	7.1	67
52	A fundamental investigation into the relationship between lubricant composition and fuel ignition quality. *Fuel*, **2015**, 160, 605-613	7.1	30
51	TG/DTG, FT-ICR Mass Spectrometry, and NMR Spectroscopy Study of Heavy Fuel Oil. *Energy & Fuels*, **2015**, 29, 7825-7835	4.1	62
50	A computational methodology for formulating gasoline surrogate fuels with accurate physical and chemical kinetic properties. *Fuel*, **2015**, 143, 290-300	7.1	112
49	Stabilization and structure of n-heptane tribrachial flames in axisymmetric laminar jets. *Proceedings of the Combustion Institute*, **2015**, 35, 1023-1032	5.9	5
48	An experimental and modeling study of n-octanol combustion. *Proceedings of the Combustion Institute*, **2015**, 35, 419-427	5.9	72
47	Kinetics of the high-temperature combustion reactions of dibutylether using composite computational methods. *Proceedings of the Combustion Institute*, **2015**, 35, 385-392	5.9	16
46	Ignition of alkane-rich FACE gasoline fuels and their surrogate mixtures. *Proceedings of the Combustion Institute*, **2015**, 35, 249-257	5.9	124
45	Combustion chemistry of alcohols: Experimental and modeled structure of a premixed 2-methylbutanol flame. *Proceedings of the Combustion Institute*, **2015**, 35, 813-820	5.9	16

44	Prospects of 2,5-dimethylfuran as a fuel: physico-chemical and engine performance characteristics evaluation. *Journal of Material Cycles and Waste Management*, **2015**, 17, 459-464	3.4	17
43	Detection and Identification of the Keto-Hydroperoxide (HOOCH2OCHO) and Other Intermediates during Low-Temperature Oxidation of Dimethyl Ether. *Journal of Physical Chemistry A*, **2015**, 119, 7361-74	2.8	111
42	Chemical kinetic study of a novel lignocellulosic biofuel: Di-n-butyl ether oxidation in a laminar flow reactor and flames. *Combustion and Flame*, **2014**, 161, 798-809	5.3	71
41	Intermediate temperature heat release in an HCCI engine fueled by ethanol/n-heptane mixtures: An experimental and modeling study. *Combustion and Flame*, **2014**, 161, 680-695	5.3	78
40	PAH growth initiated by propargyl addition: mechanism development and computational kinetics. *Journal of Physical Chemistry A*, **2014**, 118, 2865-85	2.8	58
39	Alcohol combustion chemistry. *Progress in Energy and Combustion Science*, **2014**, 44, 40-102	33.6	534
38	A comprehensive combustion chemistry study of 2,5-dimethylhexane. *Combustion and Flame*, **2014**, 161, 1444-1459	5.3	71
37	Development and validation of an n-dodecane skeletal mechanism for spray combustion applications. *Combustion Theory and Modelling*, **2014**, 18, 187-203	1.5	105
36	A counterflow diffusion flame study of branched octane isomers. *Proceedings of the Combustion Institute*, **2013**, 34, 1015-1023	5.9	39
35	On the High-Temperature Combustion of n-Butanol: Shock Tube Data and an Improved Kinetic Model. *Energy & Fuels*, **2013**, 27, 7072-7080	4.1	27
34	Detailed chemical kinetic modeling of the effects of CC double bonds on the ignition of biodiesel fuels. *Proceedings of the Combustion Institute*, **2013**, 34, 3049-3056	5.9	71
33	A comprehensive experimental and modeling study of iso-pentanol combustion. *Combustion and Flame*, **2013**, 160, 2712-2728	5.3	77
32	An experimental and modeling study investigating the ignition delay in a military diesel engine running hexadecane (cetane) fuel. *International Journal of Engine Research*, **2013**, 14, 57-67	2.7	9
31	Autoignition Characterization of Primary Reference Fuels and n-Heptane/n-Butanol Mixtures in a Constant Volume Combustion Device and Homogeneous Charge Compression Ignition Engine. *Energy & Fuels*, **2013**, 27, 7778-7789	4.1	33
30	Jet-stirred reactor and flame studies of propanal oxidation. *Proceedings of the Combustion Institute*, **2013**, 34, 599-606	5.9	33
29	An experimental and modeling study of the autoignition of 3-methylheptane. *Proceedings of the Combustion Institute*, **2013**, 34, 335-343	5.9	29
28	Experimental and modeling study of the oxidation of n- and iso-butanal. *Combustion and Flame*, **2013**, 160, 1609-1626	5.3	33
27	Computational study of the combustion and atmospheric decomposition of 2-methylfuran. *Journal of Physical Chemistry A*, **2013**, 117, 7670-85	2.8	46

26	Ignition of non-premixed counterflow flames of octane and decane isomers. *Proceedings of the Combustion Institute*, **2013**, 34, 903-910	5.9	26
25	CloudFlame: Cyberinfrastructure for Combustion Research **2013**,		7
24	Atmospheric pressure chemical ionization Fourier transform ion cyclotron resonance mass spectrometry for complex thiophenic mixture analysis. *Rapid Communications in Mass Spectrometry*, **2013**, 27, 2432-8	2.2	20
23	Modeling the combustion of high molecular weight fuels by a functional group approach. *International Journal of Chemical Kinetics*, **2012**, 44, 257-276	1.4	19
22	Experimental and Kinetic Modeling Study of 3-Methylheptane in a Jet-Stirred Reactor. *Energy & Fuels*, **2012**, 26, 4680-4689	4.1	24
21	Detailed Kinetic Modeling Study of n-Pentanol Oxidation. *Energy & Fuels*, **2012**, 26, 6678-6685	4.1	84
20	A reduced mechanism for biodiesel surrogates for compression ignition engine applications. *Fuel*, **2012**, 99, 143-153	7.1	108
19	Effects of fuel branching on the propagation of octane isomers flames. *Combustion and Flame*, **2012**, 159, 1426-1436	5.3	79
18	A comprehensive chemical kinetic combustion model for the four butanol isomers. *Combustion and Flame*, **2012**, 159, 2028-2055	5.3	407
17	A shock tube and chemical kinetic modeling study of the pyrolysis and oxidation of butanols. *Combustion and Flame*, **2012**, 159, 2009-2027	5.3	79
16	Hydrotreated Renewable Jet Fuel Ignition Delay Performance in a Military Diesel Engine: An Experimental and Modeling Study **2012**,		4
15	Comprehensive chemical kinetic modeling of the oxidation of 2-methylalkanes from C7 to C20. *Combustion and Flame*, **2011**, 158, 2338-2357	5.3	387
14	Experimental and kinetic modeling of methyl octanoate oxidation in an opposed-flow diffusion flame and a jet-stirred reactor. *Proceedings of the Combustion Institute*, **2011**, 33, 1037-1043	5.9	45
13	An Approach for Formulating Surrogates for Gasoline with Application toward a Reduced Surrogate Mechanism for CFD Engine Modeling. *Energy & Fuels*, **2011**, 25, 5215-5223	4.1	223
12	Detailed chemical kinetic reaction mechanisms for soy and rapeseed biodiesel fuels. *Combustion and Flame*, **2011**, 158, 742-755	5.3	206
11	An experimental and kinetic modeling study of n-octane and 2-methylheptane in an opposed-flow diffusion flame. *Combustion and Flame*, **2011**, 158, 1277-1287	5.3	40
10	An experimental and kinetic modeling study of methyl decanoate combustion. *Proceedings of the Combustion Institute*, **2011**, 33, 399-405	5.9	71
9	An experimental and kinetic modeling study of n-butanol combustion. *Combustion and Flame*, **2009**, 156, 852-864	5.3	253

8	A chemical kinetic study of n-butanol oxidation at elevated pressure in a jet stirred reactor. *Proceedings of the Combustion Institute*, **2009**, 32, 229-237	5.9	189
7	Experimental and chemical kinetic modeling study of small methyl esters oxidation: Methyl (E)-2-butenoate and methyl butanoate. *Combustion and Flame*, **2008**, 155, 635-650	5.3	129
6	A wide-ranging kinetic modeling study of methyl butanoate combustion. *Proceedings of the Combustion Institute*, **2007**, 31, 305-311	5.9	201
5	A comparison of saturated and unsaturated C4 fatty acid methyl esters in an opposed flow diffusion flame and a jet stirred reactor. *Proceedings of the Combustion Institute*, **2007**, 31, 1015-1022	5.9	137
4	Effect of Different Fluids on Injection Strategies to Suppress Pre-Ignition		11
3	Knock, Auto-Ignition and Pre-Ignition Tendency of Fuels for Advanced Combustion Engines (FACE) with Ethanol Blends and Similar RON		1
2	Hydrogen Selective Catalytic Reduction of Nitrogen Oxide on Pt- and Pd-Based Catalysts for Lean-Burn Automobile Applications		1
1	Predicting Ignition Quality of Oxygenated Fuels Using Artificial Neural Networks. *SAE International Journal of Fuels and Lubricants*,14,	1.8	4