S Mani Sarathy

List of Publications by Citations

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	Alcohol combustion chemistry. *Progress in Energy and Combustion Science*, **2014**, 44, 40-102	33.6	534
276	A comprehensive chemical kinetic combustion model for the four butanol isomers. *Combustion and Flame*, **2012**, 159, 2028-2055	5.3	407
275	Comprehensive chemical kinetic modeling of the oxidation of 2-methylalkanes from C7 to C20. *Combustion and Flame*, **2011**, 158, 2338-2357	5.3	387
274	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
273	An experimental and kinetic modeling study of n-butanol combustion. *Combustion and Flame*, **2009**, 156, 852-864	5.3	253
272	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
271	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
270	A comprehensive experimental and modeling study of isobutene oxidation. *Combustion and Flame*, **2016**, 167, 353-379	5.3	220
269	Recent progress in gasoline surrogate fuels. *Progress in Energy and Combustion Science*, **2018**, 65, 67-108	33.6	215
268	Detailed chemical kinetic reaction mechanisms for soy and rapeseed biodiesel fuels. *Combustion and Flame*, **2011**, 158, 742-755	5.3	206
267	A wide-ranging kinetic modeling study of methyl butanoate combustion. *Proceedings of the Combustion Institute*, **2007**, 31, 305-311	5.9	201
266	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
265	Compositional effects on the ignition of FACE gasolines. *Combustion and Flame*, **2016**, 169, 171-193	5.3	139
264	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
263	A comprehensive iso-octane combustion model with improved thermochemistry and chemical kinetics. *Combustion and Flame*, **2017**, 178, 111-134	5.3	130
262	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
261	Ignition of alkane-rich FACE gasoline fuels and their surrogate mixtures. *Proceedings of the Combustion Institute*, **2015**, 35, 249-257	5.9	124

260	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
259	A computational methodology for formulating gasoline surrogate fuels with accurate physical and chemical kinetic properties. *Fuel*, **2015**, 143, 290-300	7.1	112
258	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
257	A reduced mechanism for biodiesel surrogates for compression ignition engine applications. *Fuel*, **2012**, 99, 143-153	7.1	108
256	Development and validation of an n-dodecane skeletal mechanism for spray combustion applications. *Combustion Theory and Modelling*, **2014**, 18, 187-203	1.5	105
255	Optimized reaction mechanism rate rules for ignition of normal alkanes. *Combustion and Flame*, **2016**, 173, 468-482	5.3	96
254	Detailed Kinetic Modeling Study of n-Pentanol Oxidation. *Energy & Fuels*, **2012**, 26, 6678-6685	4.1	84
253	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
252	Effects of fuel branching on the propagation of octane isomers flames. *Combustion and Flame*, **2012**, 159, 1426-1436	5.3	79
251	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
250	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
249	Chemical Kinetic Insights into the Octane Number and Octane Sensitivity of Gasoline Surrogate Mixtures. *Energy & Fuels*, **2017**, 31, 1945-1960	4.1	77
248	A comprehensive experimental and modeling study of iso-pentanol combustion. *Combustion and Flame*, **2013**, 160, 2712-2728	5.3	77
247	An experimental and modeling study of n-octanol combustion. *Proceedings of the Combustion Institute*, **2015**, 35, 419-427	5.9	72
246	Additional chain-branching pathways in the low-temperature oxidation of branched alkanes. *Combustion and Flame*, **2016**, 164, 386-396	5.3	72
245	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
244	A comprehensive combustion chemistry study of 2,5-dimethylhexane. *Combustion and Flame*, **2014**, 161, 1444-1459	5.3	71
243	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

242	An experimental and kinetic modeling study of methyl decanoate combustion. *Proceedings of the Combustion Institute*, **2011**, 33, 399-405	5.9	71
241	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
240	Predicting Octane Number Using Nuclear Magnetic Resonance Spectroscopy and Artificial Neural Networks. *Energy & Fuels*, **2018**, 32, 6309-6329	4.1	68
239	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
238	TG/DTG, FT-ICR Mass Spectrometry, and NMR Spectroscopy Study of Heavy Fuel Oil. *Energy & Fuels*, **2015**, 29, 7825-7835	4.1	62
237	Predicting Fuel Ignition Quality Using 1H NMR Spectroscopy and Multiple Linear Regression. *Energy & Fuels*, **2016**, 30, 9819-9835	4.1	60
236	PAH growth initiated by propargyl addition: mechanism development and computational kinetics. *Journal of Physical Chemistry A*, **2014**, 118, 2865-85	2.8	58
235	An extensive experimental and modeling study of 1-butene oxidation. *Combustion and Flame*, **2017**, 181, 198-213	5.3	57
234	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
233	Third O2 addition reactions promote the low-temperature auto-ignition of n-alkanes. *Combustion and Flame*, **2016**, 165, 364-372	5.3	55
232	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
231	A blending rule for octane numbers of PRFs and TPRFs with ethanol. *Fuel*, **2016**, 180, 175-186	7.1	54
230	Optimization of the octane response of gasoline/ethanol blends. *Applied Energy*, **2017**, 203, 778-793	10.7	51
229	Autoignition characteristics of oxygenated gasolines. *Combustion and Flame*, **2017**, 186, 114-128	5.3	50
228	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
227	The site effect on PAHs formation in HACA-based mass growth process. *Combustion and Flame*, **2019**, 199, 54-68	5.3	48
226	Kinetics of ethylcyclohexane pyrolysis and oxidation: An experimental and detailed kinetic modeling study. *Combustion and Flame*, **2015**, 162, 2873-2892	5.3	47
225	A minimalist functional group (MFG) approach for surrogate fuel formulation. *Combustion and Flame*, **2018**, 192, 250-271	5.3	47

224	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
223	Computational study of the combustion and atmospheric decomposition of 2-methylfuran. *Journal of Physical Chemistry A*, **2013**, 117, 7670-85	2.8	46
222	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
221	Ignition delay measurements of light naphtha: A fully blended low octane fuel. *Proceedings of the Combustion Institute*, **2017**, 36, 315-322	5.9	44
220	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
219	Ignition studies of two low-octane gasolines. *Combustion and Flame*, **2017**, 185, 152-159	5.3	43
218	Structural Level Characterization of Base Oils Using Advanced Analytical Techniques. *Energy & Fuels*, **2015**, 29, 2962-2970	4.1	41
217	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
216	A computational study of ethylene□air sooting flames: Effects of large polycyclic aromatic hydrocarbons. *Combustion and Flame*, **2016**, 163, 427-436	5.3	39
215	A counterflow diffusion flame study of branched octane isomers. *Proceedings of the Combustion Institute*, **2013**, 34, 1015-1023	5.9	39
214	Cyclopentane combustion chemistry. Part I: Mechanism development and computational kinetics. *Combustion and Flame*, **2017**, 183, 358-371	5.3	38
213	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
212	Cyclopentane combustion. Part II. Ignition delay measurements and mechanism validation. *Combustion and Flame*, **2017**, 183, 372-385	5.3	36
211	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
210	Lifecycle optimized ethanol-gasoline blends for turbocharged engines. *Applied Energy*, **2016**, 181, 38-53	10.7	35
209	Numerical investigation of injector geometry effects on fuel stratification in a GCI engine. *Fuel*, **2018**, 214, 580-589	7.1	35
208	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
207	Development of a reduced four-component (toluene/n-heptane/iso-octane/ethanol) gasoline surrogate model. *Fuel*, **2019**, 247, 164-178	7.1	33

206	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
205	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
204	Jet-stirred reactor and flame studies of propanal oxidation. *Proceedings of the Combustion Institute*, **2013**, 34, 599-606	5.9	33
203	Experimental and modeling study of the oxidation of n- and iso-butanal. *Combustion and Flame*, **2013**, 160, 1609-1626	5.3	33
202	Chemical kinetic insights into the ignition dynamics of n-hexane. *Combustion and Flame*, **2018**, 188, 28-40	5.3	32
201	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
200	Computational study of polycyclic aromatic hydrocarbons growth by vinylacetylene addition. *Combustion and Flame*, **2019**, 202, 276-291	5.3	31
199	Three-stage heat release in n-heptane auto-ignition. *Proceedings of the Combustion Institute*, **2019**, 37, 485-492	5.9	31
198	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
197	A fundamental investigation into the relationship between lubricant composition and fuel ignition quality. *Fuel*, **2015**, 160, 605-613	7.1	30
196	Aromatic ring formation in opposed-flow diffusive 1,3-butadiene flames. *Proceedings of the Combustion Institute*, **2017**, 36, 947-955	5.9	30
195	New insights into the low-temperature oxidation of 2-methylhexane. *Proceedings of the Combustion Institute*, **2017**, 36, 373-382	5.9	30
194	Characterization of deasphalted heavy fuel oil using APPI (+) FT-ICR mass spectrometry and NMR spectroscopy. *Fuel*, **2019**, 253, 950-963	7.1	29
193	An experimental and modeling study of the autoignition of 3-methylheptane. *Proceedings of the Combustion Institute*, **2013**, 34, 335-343	5.9	29
192	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
191	Exploring gasoline oxidation chemistry in jet stirred reactors. *Fuel*, **2019**, 236, 1282-1292	7.1	29
190	A comprehensive experimental and modeling study of 2-methylbutanol combustion. *Combustion and Flame*, **2015**, 162, 2166-2176	5.3	28
189	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

188	A technological roadmap to the ammonia energy economy: Current state and missing technologies. *Chemical Engineering Journal*, **2021**, 408, 127310	14.7	28
187	Estimating fuel octane numbers from homogeneous gas-phase ignition delay times. *Combustion and Flame*, **2018**, 188, 307-323	5.3	28
186	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
185	Effects of methyl substitution on the auto-ignition of C16 alkanes. *Combustion and Flame*, **2016**, 164, 259-269	5.3	27
184	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
183	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
182	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
181	Ignition of non-premixed counterflow flames of octane and decane isomers. *Proceedings of the Combustion Institute*, **2013**, 34, 903-910	5.9	26
180	Performance and emissions of gasoline blended with terpineol as an octane booster. *Renewable Energy*, **2017**, 101, 1087-1093	8.1	26
179	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
178	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
177	Ignition characteristics of 2-methyltetrahydrofuran: An experimental and kinetic study. *Proceedings of the Combustion Institute*, **2017**, 36, 587-595	5.9	24
176	Terpineol as a novel octane booster for extending the knock limit of gasoline. *Fuel*, **2017**, 187, 9-15	7.1	24
175	Experimental and Kinetic Modeling Study of 3-Methylheptane in a Jet-Stirred Reactor. *Energy & Fuels*, **2012**, 26, 4680-4689	4.1	24
174	Jet-stirred reactor oxidation of alkane-rich FACE gasoline fuels. *Proceedings of the Combustion Institute*, **2017**, 36, 517-524	5.9	23
173	New insights into methane-oxygen ion chemistry. *Proceedings of the Combustion Institute*, **2017**, 36, 1213-1221	5.9	22
172	Machine Learning To Predict Standard Enthalpy of Formation of Hydrocarbons. *Journal of Physical Chemistry A*, **2019**, 123, 8305-8313	2.8	22
171	Methylcyclohexane pyrolysis and oxidation in a jet-stirred reactor. *Proceedings of the Combustion Institute*, **2019**, 37, 409-417	5.9	22

170	PAH formation from jet stirred reactor pyrolysis of gasoline surrogates. *Combustion and Flame*, **2020**, 219, 312-326	5.3	21
169	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
168	Evolution of oxygenated polycyclic aromatic hydrocarbon chemistry at flame temperatures. *Combustion and Flame*, **2019**, 209, 441-451	5.3	21
167	Low temperature autoignition of 5-membered ring naphthenes: Effects of substitution. *Combustion and Flame*, **2019**, 200, 387-404	5.3	21
166	One-step conversion of crude oil to light olefins using a multi-zone reactor. *Nature Catalysis*, **2021**, 4, 233-241	36.5	21
165	Improved combustion kinetic model and HCCI engine simulations of di-isopropyl ketone ignition. *Fuel*, **2016**, 164, 141-150	7.1	20
164	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
163	Chemical Ignition Characteristics of Ethanol Blending with Primary Reference Fuels. *Energy & Fuels*, **2019**, 33, 10185-10196	4.1	20
162	An experimental and modeling study of diethyl carbonate oxidation. *Combustion and Flame*, **2015**, 162, 1395-1405	5.3	20
161	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
160	2-Methylfuran: A bio-derived octane booster for spark-ignition engines. *Fuel*, **2018**, 225, 349-357	7.1	20
159	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
158	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
157	Autoignition of straight-run naphtha: A promising fuel for advanced compression ignition engines. *Combustion and Flame*, **2018**, 189, 337-346	5.3	20
156	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
155	CH4/air homogeneous autoignition: A comparison of two chemical kinetics mechanisms. *Fuel*, **2018**, 223, 74-85	7.1	19
154	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
153	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

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	Bridging the gap in a resource and climate-constrained world with advanced gasoline compression-ignition hybrids. *Applied Energy*, **2020**, 267, 114936	10.7	18
150	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
149	Simulating HCCI Blending Octane Number of Primary Reference Fuel with Ethanol **2017**,		17
148	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
147	Quantities of Interest in Jet Stirred Reactor Oxidation of a High-Octane Gasoline. *Energy & Fuels*, **2017**, 31, 5543-5553	4.1	16
146	The influence of chemical composition on ignition delay times of gasoline fractions. *Combustion and Flame*, **2019**, 209, 418-429	5.3	16
145	Ion chemistry in premixed rich methane flames. *Combustion and Flame*, **2019**, 202, 208-218	5.3	16
144	Numerical modelling of ion transport in flames. *Combustion Theory and Modelling*, **2015**, 19, 744-772	1.5	16
143	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
142	Cool diffusion flames of butane isomers activated by ozone in the counterflow. *Combustion and Flame*, **2018**, 191, 175-186	5.3	16
141	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
140	On the distillation of waste tire pyrolysis oil: A structural characterization of the derived fractions. *Fuel*, **2021**, 290, 120041	7.1	16
139	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
138	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
137	CO2 Derived E-Fuels: Research Trends, Misconceptions, and Future Directions. *Trends in Chemistry*, **2020**, 2, 785-795	14.8	15
136	Mixing-structure relationship in jet-stirred reactors. *Chemical Engineering Research and Design*, **2016** , 111, 461-464	5.5	15
135	Auto-ignition of direct injection spray of light naphtha, primary reference fuels, gasoline and gasoline surrogate. *Energy*, **2019**, 170, 375-390	7.9	15

134	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
133	Ignition delay time sensitivity in ignition quality tester (IQT) and its relation to octane sensitivity. *Fuel*, **2018**, 233, 412-419	7.1	15
132	Shock tube and modeling study of 2,7-dimethyloctane pyrolysis and oxidation. *Combustion and Flame*, **2015**, 162, 2296-2306	5.3	14
131	Spray combustion simulation study of waste cooking oil biodiesel and diesel under direct injection diesel engine conditions. *Fuel*, **2020**, 267, 117240	7.1	14
130	High-Pressure Limit Rate Rules for □H Isomerization of Hydroperoxyalkylperoxy Radicals. *Journal of Physical Chemistry A*, **2018**, 122, 3626-3639	2.8	14
129	Effects of Substitution on Counterflow Ignition and Extinction of C3 and C4 Alcohols. *Energy & Fuels*, **2016**, 30, 6091-6097	4.1	14
128	Effect of Mixture Formation and Injection Strategies on Stochastic Pre-Ignition **2018**,		14
127	Combustion chemistry of ammonia/hydrogen mixtures: Jet-stirred reactor measurements and comprehensive kinetic modeling. *Combustion and Flame*, **2021**, 234, 111653	5.3	14
126	Experiments and simulations of NOx formation in the combustion of hydroxylated fuels. *Combustion and Flame*, **2015**, 162, 2322-2336	5.3	13
125	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
124	Global sensitivity analysis of n-butanol reaction kinetics using rate rules. *Combustion and Flame*, **2018**, 196, 452-465	5.3	13
123	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
122	Experimental and Numerical Investigation of Ethanol/Diethyl Ether Mixtures in a CI Engine **2016**,		13
121	Automated chemical kinetic mechanism simplification with minimal user expertise. *Combustion and Flame*, **2018**, 197, 439-448	5.3	13
120	Rapid soot inception via □alkynyl substitution of polycyclic aromatic hydrocarbons. *Fuel*, **2021**, 295, 120580	7.1	13
119	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
118	Enhanced lubrication by core-shell TiO2 nanoparticles modified with gallic acid ester. *Tribology International*, **2020**, 146, 106263	4.9	12
117	Understanding premixed flame chemistry of gasoline fuels by comparing quantities of interest. *Proceedings of the Combustion Institute*, **2017**, 36, 1203-1211	5.9	12

116	Two-stage Lagrangian modeling of ignition processes in ignition quality tester and constant volume combustion chambers. *Fuel*, **2016**, 185, 589-598	7.1	12
115	A comprehensive experimental and kinetic modeling study of 1- and 2-pentene. *Combustion and Flame*, **2021**, 223, 166-180	5.3	12
114	Ab Initio, Transition State Theory, and Kinetic Modeling Study of the HO-Assisted Keto-Enol Tautomerism Propen-2-ol + HO <ɑAcetone + HO under Combustion, Atmospheric, and Interstellar Conditions. *Journal of Physical Chemistry A*, **2018**, 122, 9792-9805	2.8	12
113	Variations in non-thermal NO formation pathways in alcohol flames. *Proceedings of the Combustion Institute*, **2017**, 36, 3995-4002	5.9	11
112	Premixed flame chemistry of a gasoline primary reference fuel surrogate. *Combustion and Flame*, **2017**, 179, 300-311	5.3	11
111	Achieving 80% greenhouse gas reduction target in Saudi Arabia under low and medium oil prices. *Energy Policy*, **2017**, 101, 502-511	7.2	11
110	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
109	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
108	Effect of Different Fluids on Injection Strategies to Suppress Pre-Ignition		11
107	Efficient alkane oxidation under combustion engine and atmospheric conditions. *Communications Chemistry*, **2021**, 4,	6.3	11
106	Measurements of Positively Charged Ions in Premixed Methane-Oxygen Atmospheric Flames. *Combustion Science and Technology*, **2017**, 189, 575-594	1.5	10
105	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
104	Reduced Gasoline Surrogate (Toluene/n-Heptane/iso-Octane) Chemical Kinetic Model for Compression Ignition Simulations **2018**,		10
103	Autoignition of diethyl ether and a diethyl ether/ethanol blend. *Fuel*, **2020**, 279, 118553	7.1	9
102	A surrogate fuel formulation to characterize heating and evaporation of light naphtha droplets. *Combustion Science and Technology*, **2018**, 190, 1218-1231	1.5	9
101	Experimental and Chemical Kinetic Modeling Study of Dimethylcyclohexane Oxidation and Pyrolysis. *Energy & Fuels*, **2016**, 30, 8648-8657	4.1	9
100	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
99	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

98	Effectiveness of Fuel Enrichment on Knock Suppression in a Gasoline Spark-Ignited Engine **2018**,		9
97	Ethanolic gasoline, a lignocellulosic advanced biofuel. *Sustainable Energy and Fuels*, **2019**, 3, 409-421	5.8	8
96	Autoignition Characteristics of Ethers Blended with Low Cetane Distillates. *Energy & Fuels*, **2019**, 33, 6775-6787	4.1	8
95	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
94	Blending Behavior of Ethanol with PRF 84 and FACE A Gasoline in HCCI Combustion Mmode **2017**,		8
93	Techno-Economic Analysis of Pressurized Oxy-Fuel Combustion of Petroleum Coke. *Energies*, **2020**, 13, 3463	3.1	8
92	Pinene - A High Energy Density Biofuel for SI Engine Applications **2016**,		8
91	A functional-group-based approach to modeling real-fuel combustion chemistry : Prediction of stoichiometric parameters for lumped pyrolysis reactions. *Combustion and Flame*, **2021**, 227, 497-509	5.3	8
90	Probing the Chemical Kinetics of Minimalist Functional Group Gasoline Surrogates. *Energy & Fuels*, **2021**, 35, 3315-3332	4.1	8
89	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
88	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
87	CloudFlame: Cyberinfrastructure for Combustion Research **2013**,		7
86	Data Science Approach to Estimate Enthalpy of Formation of Cyclic Hydrocarbons. *Journal of Physical Chemistry A*, **2020**, 124, 6270-6276	2.8	7
85	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
84	Computational singular perturbation analysis of brain lactate metabolism. *PLoS ONE*, **2019**, 14, e0226094	3.7	7
83	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
82	Unraveling the octane response of gasoline/ethanol blends: Paving the way to formulating gasoline surrogates. *Fuel*, **2021**, 299, 120882	7.1	7
81	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

80	Gas-to-Liquid Phase Transition of PAH at Flame Temperatures. *Journal of Physical Chemistry A*, **2020**, 124, 3896-3903	2.8	6
79	Screening gas-phase chemical kinetic models: Collision limit compliance and ultrafast timescales. *International Journal of Chemical Kinetics*, **2020**, 52, 599-610	1.4	6
78	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
77	Chemical kinetics of hydroxyl reactions with cyclopentadiene and indene. *Combustion and Flame*, **2020**, 217, 48-56	5.3	6
76	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
75	A droplet reactor on a super-hydrophobic surface allows control and characterization of amyloid fibril growth. *Communications Biology*, **2020**, 3, 457	6.7	6
74	Environmental Challenges and Opportunities in Marine Engine Heavy Fuel Oil Combustion. *Lecture Notes in Civil Engineering*, **2019**, 1047-1055	0.3	6
73	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
72	Stabilization and structure of n-heptane tribrachial flames in axisymmetric laminar jets. *Proceedings of the Combustion Institute*, **2015**, 35, 1023-1032	5.9	5
71	Lube Products: Molecular Characterization of Base Oils **2018**, 1-14		5
70	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
69	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
68	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
67	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
66	Exploring low temperature oxidation of 1-butene in jet-stirred reactors. *Combustion and Flame*, **2020**, 222, 259-271	5.3	5
65	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
64	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
63	Ignition delay time measurements of diesel and gasoline blends. *Combustion and Flame*, **2020**, 222, 460-475	5.3	5

62	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
61	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
60	Fuel Class Higher Alcohols **2016**, 29-57		5
59	A theoretical study of the H- and HO□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
58	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
57	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
56	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
55	Identification of volatile constituents released from IQOS heat-not-burn tobacco HeatSticks using a direct sampling method. *Tobacco Control*, **2020**,	5.3	4
54	Hydrotreated Renewable Jet Fuel Ignition Delay Performance in a Military Diesel Engine: An Experimental and Modeling Study **2012**,		4
53	High purity, self-sustained, pressurized hydrogen production from ammonia in a catalytic membrane reactor. *Chemical Engineering Journal*, **2022**, 431, 134310	14.7	4
52	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
51	Predicting Ignition Quality of Oxygenated Fuels Using Artificial Neural Networks. *SAE International Journal of Fuels and Lubricants*,14,	1.8	4
50	Polyether-Based Block Co(ter)polymers as Multifunctional Lubricant Additives. *ACS Applied Polymer Materials*, **2021**, 3, 3811-3820	4.3	4
49	Oxidative-Coupling-Assisted Methane Aromatization: A Simulation Study. *Industrial & Engineering Chemistry Research*, **2019**, 58, 22884-22892	3.9	4
48	Chemical structure of atmospheric pressure premixed laminar formic acid/hydrogen flames. *Proceedings of the Combustion Institute*, **2021**, 38, 2379-2386	5.9	4
47	Simultaneous production of ketohydroperoxides from low temperature oxidation of a gasoline primary reference fuel mixture. *Fuel*, **2021**, 288, 119737	7.1	4
46	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
45	A comprehensive combustion chemistry study of n-propylcyclohexane. *Combustion and Flame*, **2021**, 233, 111576	5.3	4

44	Impact of thermodynamic properties and heat loss on ignition of transportation fuels in rapid compression machines. *Fuel*, **2018**, 218, 203-212	7.1	3
43	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
42	A comprehensive neural network model for predicting flash point of oxygenated fuels using a functional group approach. *Fuel*, **2022**, 317, 123428	7.1	3
41	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
40	Investigating Water Injection in Single-Cylinder Gasoline Spark-Ignited Engines at Fixed Speed. *Energy & Fuels*, **2020**, 34, 16636-16653	4.1	3
39	Predicting entropy and heat capacity of hydrocarbons using machine learning. *Energy and AI*, **2021**, 4, 100054	12.6	3
38	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
37	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
36	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
35	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
34	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
33	Noncatalytic Oxidative Coupling of Methane (OCM): Gas-Phase Reactions in a Jet Stirred Reactor (JSR).. *ACS Omega*, **2021**, 6, 33757-33768	3.9	2
32	On the effects of CO2 atmosphere in the pyrolysis of Salicornia bigelovii. *Bioresource Technology Reports*, **2022**, 17, 100950	4.1	2
31	Ammonia and ammonia/hydrogen blends oxidation in a jet-stirred reactor: Experimental and numerical study. *Fuel*, **2022**, 310, 122202	7.1	2
30	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
29	Understanding the synergistic blending octane behavior of 2-methylfuran. *Proceedings of the Combustion Institute*, **2021**, 38, 5625-5633	5.9	2
28	Effects of ammonia addition on soot formation in ethylene laminar premixed flames. *Combustion and Flame*, **2021**, 111698	5.3	2
27	On the origins of lubricity and surface cleanliness in ethanol-diesel fuel blends. *Fuel*, **2021**, 302, 121135	7.1	2

26	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
25	The impact of gasoline formulation on turbulent jet ignition. *Fuel*, **2022**, 324, 124373	7.1	2
24	Chemical kinetic study of triptane (2,2,3-trimethylbutane) as an anti-knock additive. *Combustion and Flame*, **2019**, 210, 399-412	5.3	1
23	Optimizing Blendstock Composition and Ethanol Feedstock to Reduce Gasoline Well-to-Pump CO 2 Emission. *Energy Procedia*, **2017**, 105, 3642-3647	2.3	1
22	Knock, Auto-Ignition and Pre-Ignition Tendency of Fuels for Advanced Combustion Engines (FACE) with Ethanol Blends and Similar RON		1
21	Hydrogen Selective Catalytic Reduction of Nitrogen Oxide on Pt- and Pd-Based Catalysts for Lean-Burn Automobile Applications		1
20	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
19	Theoretical Study of an Undisclosed Reaction Class: Direct H-Atom Abstraction from Allylic Radicals by Molecular Oxygen. *Energies*, **2021**, 14, 2916	3.1	1
18	Using deep neural networks to diagnose engine pre-ignition. *Proceedings of the Combustion Institute*, **2021**, 38, 5915-5922	5.9	1
17	Counterflow ignition and extinction of FACE gasoline fuels. *Proceedings of the Combustion Institute*, **2021**, 38, 2323-2331	5.9	1
16	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
15	Atomistic simulations of syngas oxy-combustion in supercritical CO2. *Journal of CO2 Utilization*, **2021**, 49, 101554	7.6	1
14	Hydrogen Evolution from Hydrocarbon Pyrolysis in a Simulated Liquid Metal Bubble Reactor. *Energy & Fuels*, **2021**, 35, 14597-14609	4.1	1
13	Probing the gas-phase oxidation of ammonia: Addressing uncertainties with theoretical calculations. *Combustion and Flame*, **2021**, 111708	5.3	1
12	A reinforcement learning-based economic model predictive control framework for autonomous operation of chemical reactors. *Chemical Engineering Journal*, **2022**, 428, 130993	14.7	1
11	A Methodology for Designing Octane Number of Fuels Using Genetic Algorithms and Artificial Neural Networks. *Energy & Fuels*, **2022**, 36, 3867-3880	4.1	1
10	Revisiting low temperature oxidation chemistry of n-heptane. *Combustion and Flame*, **2022**, 242, 112177	5.3	1
9	Investigating the Effects of C3 and C4 Alcohol Blending on Ignition Quality of Gasoline Fuels. *Energy & Fuels*, **2020**, 34, 8777-8787	4.1	0

8	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
7	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
6	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
5	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
4	Accurate thermochemistry prediction of extensive Polycyclic aromatic hydrocarbons (PAHs) and relevant radicals. *Combustion and Flame*, **2022**, 242, 112159	5.3	0
3	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
2	Artificial intelligence-enabled fuel design **2022**, 47-67		
1	On the lubricity mechanism of carbon-based nanofluid fuels. *Fuel*, **2022**, 308, 122031	7.1	