Anthony M Dean

List of Publications by Year
in descending order

102 papers	6,244 citations	61984 43 h-index	82547 72 g-index
104 all docs	104 docs citations	104 times ranked	3343 citing authors

#	Article	IF	Citations
1	Rate rules and reaction classes. Computer Aided Chemical Engineering, 2019, 45, 203-257.	0.5	4
2	Impact of the Molecular Structure on Olefin Pyrolysis. Energy & Fuels, 2017, 31, 6515-6524.	5.1	7
3	Experimental and kinetic modeling study of butene isomer pyrolysis: Part II. Isobutene. Combustion and Flame, 2017, 176, 23-37.	5.2	21
4	Comparative Kinetic Analysis of Ethane Pyrolysis at 0.1 and 2.0 MPa. Energy & Fuels, 2016, 30, 9703-9711.	5.1	8
5	Investigation of Iso-octane Ignition and Validation of a Multizone Modeling Method in an Ignition Quality Tester. Energy & Fuels, 2016, 30, 9761-9771.	5.1	14
6	Experimental and kinetic modeling study of butene isomer pyrolysis: Part I. 1- and 2-Butene. Combustion and Flame, 2016, 173, 347-369.	5.2	31
7	Chemical Kinetics: A CS Perspective. Computing in Science and Engineering, 2016, 18, 48-55.	1.2	0
8	Ab initio study of the influence of resonance stabilization on intramolecular ring closure reactions of hydrocarbon radicals. Physical Chemistry Chemical Physics, 2016, 18, 8437-8452.	2.8	20
9	The impact of fuel evaporation on the gas-phase kinetics in the mixing region of a diesel autothermal reformer. International Journal of Hydrogen Energy, 2015, 40, 15477-15490.	7.1	9
10	Impact of Finite Mixing on Gas-Phase Partial Oxidation for Selective Removal of Deposit Precursors from Gasifier Outlet Streams. Energy & Fuels, 2015, 29, 6501-6511.	5.1	1
11	The Impact of Resonance Stabilization on the Intramolecular Hydrogenâ€Atom Shift Reactions of Hydrocarbon Radicals. ChemPhysChem, 2015, 16, 2635-2645.	2.1	21
12	Reactions of allylic radicals that impact molecular weight growth kinetics. Physical Chemistry Chemical Physics, 2015, 17, 6255-6273.	2.8	49
13	Reactivityâ€“Structure-Based Rate Estimation Rules for Alkyl Radical H Atom Shift and Alkenyl Radical Cycloaddition Reactions. Journal of Physical Chemistry A, 2015, 119, 7205-7221.	2.5	60
14	A comparison of H2S, SO2, and COS poisoning on Ni/YSZ and Ni/K2O-CaAl2O4 during methane steam and dry reforming. Applied Catalysis A: General, 2015, 502, 399-409.	4.3	44
15	Fundamentally-based kinetic model for propene pyrolysis. Combustion and Flame, 2015, 162, 4456-4470.	5.2	57
16	Unravelling the impact of hydrocarbon structure on the fumarate addition mechanism â€“ a gas-phaseab initiostudy. Physical Chemistry Chemical Physics, 2015, 17, 4054-4066.	2.8	14
17	Experiments and Computational Fluid Dynamics Modeling Analysis of Large n-Alkane Ignition Kinetics in the Ignition Quality Tester. Energy & Fuels, 2014, 28, 4781-4794.	5.1	35
18	Model-predicted effects of fuel droplet diameter and <mml:math altimg="si10.gif" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xmlns:ce="ht. Combustion and Flame,	5.2	1

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19	Insights into the Glycyl Radical Enzyme Active Site of Benzylsuccinate Synthase: A Computational Study. Journal of the American Chemical Society, 2013, 135, 12279-12288.	13.7	30
20	Rate Rules, Branching Ratios, and Pressure Dependence of the HO₂ + Olefin Addition Channels. Journal of Physical Chemistry A, 2013, 117, 6458-6473.	2.5	57
21	The effects of multicomponent fuel droplet evaporation on the kinetics of strained opposed-flow diffusion flames. Combustion and Flame, 2013, 160, 265-275.	5.2	23
22	RCARM: Reaction classification using automated reaction mapping. International Journal of Chemical Kinetics, 2013, 45, 125-139.	1.6	4
23	Ignition Quality Tester (IQT) Investigation of the Negative Temperature Coefficient Region of Alkane Autoignition. Energy & Fuels, 2013, 27, 1632-1642.	5.1	56
24	Coupled transport and kinetics in the mixing region for hydrocarbon autothermal reforming applications. International Journal of Hydrogen Energy, 2013, 38, 16140-16151.	7.1	7
25	Simulation of n-Heptane and Surrogate Fuels for Advanced Combustion Engines (FACE) in a Single-Cylinder Compression Ignition Engine. , 2013, , .		2
26	High-Pressure Rate Rules for Alkyl + O₂ Reactions. 2. The Isomerization, Cyclic Ether Formation, and Î²-Scission Reactions of Hydroperoxy Alkyl Radicals. Journal of Physical Chemistry A, 2012, 116, 5068-5089.	2.5	172
27	Investigation of gas-phase reactions in the mixing region for hydrocarbon autothermal reforming applications. International Journal of Hydrogen Energy, 2012, 37, 7545-7553.	7.1	8
28	A quantitative kinetic analysis of CO elimination from phenoxy radicals. International Journal of Chemical Kinetics, 2012, 44, 75-89.	1.6	40
29	Direct Detection of Products from the Pyrolysis of 2-Phenethyl Phenyl Ether. Journal of Physical Chemistry A, 2011, 115, 428-438.	2.5	160
30	Numerical and Experimental Investigation of n-Heptane Autoignition in the Ignition Quality Tester (IQT). Energy & Fuels, 2011, 25, 5562-5572.	5.1	61
31	Kinetic Modeling of Ethane Pyrolysis at High Conversion. Journal of Physical Chemistry A, 2011, 115, 10470-10490.	2.5	41
32	High-Pressure Rate Rules for Alkyl + O₂ Reactions. 1. The Dissociation, Concerted Elimination, and Isomerization Channels of the Alkyl Peroxy Radical. Journal of Physical Chemistry A, 2011, 115, 13425-13442.	2.5	223
33	Impact of gas-phase reactions in the mixing region upstream of a diesel fuel autothermal reformer. Journal of Power Sources, 2011, 196, 2020-2026.	7.8	20
34	The effects of liquid-fuel thermophysical properties, carrier-gas composition, and pressure, on strained opposed-flow non-premixed flames. Combustion and Flame, 2011, 158, 1129-1139.	5.2	18
35	Development of Detailed Kinetic Models for the Thermal Conversion of Biomass via First Principle Methods and Rate Estimation Rules. ACS Symposium Series, 2010, , 201-243.	0.5	23
36	Kinetic Analysis of C4 Alkane and Alkene Pyrolysis: Implications for SOFC Operation. Journal of Fuel Cell Science and Technology, 2010, 7, .	0.8	8

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37	Selective Removal of Ethylene, a Deposit Precursor, from a â€œDirtyâ€•Synthesis Gas Stream via Gas-Phase Partial Oxidation. Journal of Physical Chemistry A, 2010, 114, 6502-6514.	2.5	12
38	Detailed Modeling of Low-Temperature Propane Oxidation: 1. The Role of the Propyl + O₂ Reaction. Journal of Physical Chemistry A, 2010, 114, 6594-6607.	2.5	70
39	Impact of Gas-Phase Reactions on SOFC Systems Operating on Diesel and Biomass-Derived Fuels. Materials Science Forum, 2010, 638-642, 1118-1124.	0.3	2
40	Coupling Complex Reformer Chemical Kinetics with Three-Dimensional Computational Fluid Dynamics. ECS Transactions, 2009, 25, 1253-1262.	0.5	9
41	Modeling high pressure ethane oxidation and pyrolysis. Proceedings of the Combustion Institute, 2009, 32, 437-443.	3.9	11
42	Non-catalytic partial oxidation of bio-oil to synthesis gas for distributed hydrogen production. International Journal of Hydrogen Energy, 2009, 34, 8519-8534.	7.1	45
43	Rate Constant Rules for the Automated Generation of Gas-Phase Reaction Mechanisms. Journal of Physical Chemistry A, 2009, 113, 367-380.	2.5	95
44	Hydrocarbon Fuels in Solid Oxide Fuel Cells:â€‰ In Situ Raman Studies of Graphite Formation and Oxidation. Journal of Physical Chemistry C, 2008, 112, 5232-5240.	3.1	88
45	Ethanol Transport and Chemistry in Solid Oxide Fuel Cells. , 2008, , .		0
46	Hydrocarbon fuel effects in solid-oxide fuel cell operation: an experimental and modeling study of n-hexane pyrolysis. Physical Chemistry Chemical Physics, 2007, 9, 4245.	2.8	39
47	Chapter 4 The Kinetics of Pressure-Dependent Reactions. Comprehensive Chemical Kinetics, 2007, 42, 101-184.	2.3	30
48	Rate constants for the H abstraction from alkanes (Râ€“H) by Râ€²O2 radicals: A systematic study on the impact of R and Râ€². Proceedings of the Combustion Institute, 2007, 31, 149-157.	3.9	89
49	Detailed kinetic modeling of ethane oxidation. Combustion and Flame, 2006, 145, 16-37.	5.2	52
50	Gas-phase reactions of methane and natural-gas with air and steam in non-catalytic regions of a solid-oxide fuel cell. Journal of Power Sources, 2006, 156, 434-447.	7.8	50
51	Comparison of conversion and deposit formation of ethanol and butane under SOFC conditions. Journal of Power Sources, 2006, 158, 497-503.	7.8	56
52	Performance predictions of a tubular SOFC operating on a partially reformed JP-8 surrogate. Journal of Power Sources, 2006, 162, 553-562.	7.8	19
53	Rate constants for the abstraction reactions RO2+C2H6; R=H, CH3, and C2H5. Proceedings of the Combustion Institute, 2005, 30, 995-1003.	3.9	41
54	Methane reforming kinetics within a Niâ€“YSZ SOFC anode support. Applied Catalysis A: General, 2005, 295, 40-51.	4.3	290

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55	Detailed Modeling of the Reaction of C2H5+ O2. Journal of Physical Chemistry A, 2005, 109, 2264-2281.	2.5	65
56	Importance of Gas-Phase Kinetics within the Anode Channel of a Solid-Oxide Fuel Cell. Journal of Physical Chemistry A, 2004, 108, 3772-3783.	2.5	75
57	Homogeneous kinetics and equilibrium predictions of coking propensity in the anode channels of direct oxidation solid-oxide fuel cells using dry natural gas. Journal of Power Sources, 2003, 123, 182-189.	7.8	74
58	Application of Computational Kinetic Mechanism Generation to Model the Autocatalytic Pyrolysis of Methane. Industrial & Engineering Chemistry Research, 2003, 42, 1000-1010.	3.7	32
59	Mechanism Generation with Integrated Pressure Dependence:Â A New Model for Methane Pyrolysis. Journal of Physical Chemistry A, 2003, 107, 8552-8565.	2.5	94
60	Detailed Kinetics and Thermochemistry of C2H5+ O2:Â Reaction Kinetics of the Chemically-Activated and Stabilized CH3CH2OOâ€¢Adduct. Journal of Physical Chemistry A, 2002, 106, 7276-7293.	2.5	140
61	The formation of ultrathin silicon oxide films using H2/N2O mixtures. Proceedings of the Combustion Institute, 2002, 29, 1055-1062.	3.9	2
62	Computer Construction of Detailed Chemical Kinetic Models for Gas-Phase Reactors. Industrial & Engineering Chemistry Research, 2001, 40, 5362-5370.	3.7	78
63	Variational optimisation by the solution of a series of Hamiltonâ€“Jacobi equations. Physica D: Nonlinear Phenomena, 2001, 154, 15-25.	2.8	2
64	Rate-based screening of pressure-dependent reaction networks. Computer Physics Communications, 2001, 138, 237-249.	7.5	24
65	Combustion Chemistry of Nitrogen. , 2000, , 125-341.		136
66	Master equation analysis of intermolecular energy transfer in multiple-well, multiple-channel unimolecular reactions. II. Numerical methods and application to the mechanism of the C2H5+O2 reaction. Journal of Chemical Physics, 1999, 111, 8313-8329.	3.0	51
67	Hydrogen abstraction rates via density functional theory. Chemical Physics Letters, 1999, 312, 262-268.	2.6	26
68	Microcanonical Transition State Theory Rate Coefficients from Thermal Rate Constants via Inverse Laplace Transformation. Journal of Physical Chemistry A, 1998, 102, 8104-8115.	2.5	3
69	Bayesian method for global optimization. Physical Review E, 1997, 55, 6219-6232.	2.1	11
70	Master equation analysis of intermolecular energy transfer in multiple-well, multiple-channel unimolecular reactions. I. Basic theory. Journal of Chemical Physics, 1997, 107, 8904-8916.	3.0	31
71	CHEBYSHEV EXPANSIONS AND SENSITIVITY ANALYSIS FOR APPROXIMATING THE TEMPERATURE- AND PRESSURE-DEPENDENCE OF CHEMICALLY-ACTIVATED REACTIONS. Reviews in Chemical Engineering, 1997, 13, 1-67.	4.4	8
72	Rate-Based Construction of Kinetic Models for Complex Systems. Journal of Physical Chemistry A, 1997, 101, 3731-3740.	2.5	192

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73	Parameterization of pressure- and temperature-dependent kinetics in multiple well reactions. AICHE Journal, 1997, 43, 1331-1340.	3.6	40
74	Molecular density of states from estimated vapor phase heat capacities. International Journal of Chemical Kinetics, 1997, 29, 161-170.	1.6	62
75	O + NNH: A possible new route for NOX formation in flames. International Journal of Chemical Kinetics, 1995, 27, 1097-1109.	1.6	222
76	Hydrogen Atom Bond Increments for Calculation of Thermodynamic Properties of Hydrocarbon Radical Species. The Journal of Physical Chemistry, 1995, 99, 14514-14527.	2.9	160
77	Analysis of the reactions H+N2O and NH+NO: Pathways and rate constants over a wide range of temperature and pressure. Proceedings of the Combustion Institute, 1994, 25, 965-974.	0.3	35
78	The numerical solution of some kinetics models with VODE and CHEMKIN II. Computers & Chemistry, 1993, 17, 297-302.	1.2	59
79	Hydrocarbon radical reactions with oxygen: comparison of allyl, formyl, and vinyl to ethyl. The Journal of Physical Chemistry, 1993, 97, 4427-4441.	2.9	145
80	Reactions of CH2 and CH with N2 and CH with NO. , 1993, , 101-116.		3
81	CHEMACT: A Computer Code to Estimate Rate Constants for Chemically-Activated Reactions. Combustion Science and Technology, 1991, 80, 63-85.	2.3	84
82	Detailed kinetic modeling of autocatalysis in methane pyrolysis. The Journal of Physical Chemistry, 1990, 94, 1432-1439.	2.9	151
83	Kinetic study on thermal decomposition of chlorobenzene diluted in hydrogen. The Journal of Physical Chemistry, 1990, 94, 2493-2504.	2.9	110
84	Chemical activation analysis of the reaction of ethyl radical with oxygen. The Journal of Physical Chemistry, 1990, 94, 3313-3317.	2.9	107
85	Forming benzene in flames by chemically activated isomerization. The Journal of Physical Chemistry, 1989, 93, 8171-8180.	2.9	328
86	Energized complex quantum Rice-Ramsperger-Kassel analysis on reactions of amidogen with hydroperoxo, oxygen and oxygen atoms. The Journal of Physical Chemistry, 1989, 93, 1058-1065.	2.9	60
87	Bimolecular QRRK analysis of methyl radical reactions. International Journal of Chemical Kinetics, 1987, 19, 207-228.	1.6	142
88	Prediction of rate constants for combustion and pyrolysis reactions by bimolecular QRRK. AICHE Journal, 1986, 32, 1971-1979.	3.6	101
89	Excimer laser perturbations of methane flames: High temperature reactions of OH and CH. International Journal of Chemical Kinetics, 1985, 17, 1103-1118.	1.6	8
90	Kinetics of rich ammonia flames. International Journal of Chemical Kinetics, 1984, 16, 633-653.	1.6	86

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91	Laser induced fluorescence and absorption measurements of NO in NH3/O2 and CH4/air flames. Journal of Chemical Physics, 1983, 78, 5962-5970.	3.0	54
92	Nitrogen Chemistry in Flames. ACS Symposium Series, 1983, , 71-86.	0.5	13
93	Shock-tube studies of formaldehyde oxidation. Combustion and Flame, 1980, 37, 41-62.	5.2	100
94	Shock tube studies of the N2O/CH4/CO/Ar and N2O/C2H6/CO/Ar systems. Combustion and Flame, 1980, 37, 109-123.	5.2	12
95	A shock tube study of the recombination of carbon monoxide and oxygen atoms. Journal of Chemical Physics, 1977, 66, 598-604.	3.0	25
96	Shock tube studies of the N2O/Ar and N2O/H2/Ar systems. International Journal of Chemical Kinetics, 1976, 8, 459-474.	1.6	24
97	N2O Dissociation behind reflected shock waves. International Journal of Chemical Kinetics, 1975, 7, 381-398.	1.6	16
98	Reaction of atomic oxygen with carbon dioxide behind reflected shock waves. Journal of Chemical Physics, 1974, 60, 307-313.	3.0	13
99	On-Line Computer Acquisition of Data from a Shocktube Experiment*.. Instrumentation Science and Technology, 1974, 5, 109-126.	1.8	7
100	Dissociation of carbon dioxide behind reflected shock waves. Journal of Chemical Physics, 1973, 58, 5202-5208.	3.0	21
101	Mechanism of the Smokeless Rich Diesel Combustion by Reducing Temperature. , 0, , .		632
102	Expanding the Experimental Capabilities of the Ignition Quality Tester for Autoigniting Fuels. SAE International Journal of Fuels and Lubricants, 0, 3, 353-367.	0.2	31