

Michael F Doherty

List of Publications by Citations

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171
papers

7,528
citations

52
h-index

78
g-index

180
ext. papers

8,123
ext. citations

4.6
avg, IF

6.12
L-index

#	Paper	IF	Citations
171	Crystal Shape Engineering. <i>Industrial & Engineering Chemistry Research</i> , 2008 , 47, 9812-9833	3.9	250
170	Modeling crystal shapes of organic materials grown from solution. <i>AIChE Journal</i> , 2000 , 46, 1348-1367	3.6	215
169	From form to function: Crystallization of active pharmaceutical ingredients. <i>AIChE Journal</i> , 2008 , 54, 1682-1688	3.6	205
168	Reactive Distillation. <i>Industrial & Engineering Chemistry Research</i> , 2000 , 39, 3953-3957	3.9	195
167	Homogeneous nucleation of methane hydrates: unrealistic under realistic conditions. <i>Journal of the American Chemical Society</i> , 2012 , 134, 19544-7	16.4	188
166	Vapor-liquid phase equilibrium in systems with multiple chemical reactions. <i>Chemical Engineering Science</i> , 1995 , 50, 23-48	4.4	165
165	Design and minimum-reflux calculations for single-feed multicomponent reactive distillation columns. <i>Chemical Engineering Science</i> , 1988 , 43, 1523-1537	4.4	139
164	The simple distillation of homogeneous reactive mixtures. <i>Chemical Engineering Science</i> , 1988 , 43, 541-550	4.4	138
163	Design and synthesis of homogeneous azeotropic distillations. 3. The sequencing of columns for azeotropic and extractive distillations. <i>Industrial & Engineering Chemistry Fundamentals</i> , 1985 , 24, 474-485		134
162	A new pressure-swing-distillation process for separating homogeneous azeotropic mixtures. <i>Industrial & Engineering Chemistry Research</i> , 1992 , 31, 346-357	3.9	127
161	Design and synthesis of homogeneous azeotropic distillations. 2. Minimum reflux calculations for nonideal and azeotropic columns. <i>Industrial & Engineering Chemistry Fundamentals</i> , 1985 , 24, 463-474		117
160	Measurement of Residue Curve Maps and Heterogeneous Kinetics in Methyl Acetate Synthesis. <i>Industrial & Engineering Chemistry Research</i> , 1998 , 37, 1917-1928	3.9	115
159	Geometric behavior and minimum flows for nonideal multicomponent distillation. <i>Chemical Engineering Science</i> , 1990 , 45, 1801-1822	4.4	110
158	Design Method for Kinetically Controlled, Staged Reactive Distillation Columns. <i>Industrial & Engineering Chemistry Research</i> , 1998 , 37, 2821-2834	3.9	109
157	Design and synthesis of homogeneous azeotropic distillations. 1. Problem formulation for a single column. <i>Industrial & Engineering Chemistry Fundamentals</i> , 1985 , 24, 454-463		107
156	The influence of equilibrium chemical reactions on vapor-liquid phase diagrams. <i>Chemical Engineering Science</i> , 1988 , 43, 529-540	4.4	100
155	Effect of kinetics on residue curve maps for reactive distillation. <i>AIChE Journal</i> , 1994 , 40, 1814-1824	3.6	97

154	Thermal integration of homogeneous azeotropic distillation sequences. <i>AIChE Journal</i> , 1990 , 36, 969-984	3.6	97
153	Synthesis of Reactive Distillation Systems with Multiple Equilibrium Chemical Reactions. <i>Industrial & Engineering Chemistry Research</i> , 1995 , 34, 2555-2565	3.9	95
152	Regions of attainable particle sizes in continuous and batch crystallization processes. <i>Chemical Engineering Science</i> , 2014 , 106, 167-180	4.4	91
151	Engineering Crystal Morphology. <i>Annual Review of Materials Research</i> , 2013 , 43, 359-386	12.8	91
150	Global Stability Analysis and Calculation of Liquid-Liquid Equilibrium in Multicomponent Mixtures. <i>Industrial & Engineering Chemistry Research</i> , 1996 , 35, 1395-1408	3.9	90
149	A new technique for predicting the shape of solution-grown organic crystals. <i>AIChE Journal</i> , 1998 , 44, 2501-2514	3.6	84
148	Minimum entrainer flows for extractive distillation: A bifurcation theoretic approach. <i>AIChE Journal</i> , 1994 , 40, 243-268	3.6	84
147	Automatic screening of entrainers for homogeneous azeotropic distillation. <i>Industrial & Engineering Chemistry Research</i> , 1991 , 30, 760-772	3.9	82
146	Attainable regions for reaction with separation. <i>AIChE Journal</i> , 1997 , 43, 374-387	3.6	80
145	Chaos in deterministic systems: Strange attractors, turbulence, and applications in chemical engineering. <i>Chemical Engineering Science</i> , 1988 , 43, 139-183	4.4	79
144	Structure of Distillation Regions for Multicomponent Azeotropic Mixtures. <i>AIChE Journal</i> , 1998 , 44, 1382-1391	3.6	78
143	Shape evolution of 3-dimensional faceted crystals. <i>AIChE Journal</i> , 2006 , 52, 1906-1915	3.6	75
142	Modeling Crystal Shape of Polar Organic Materials: Applications to Amino Acids. <i>Crystal Growth and Design</i> , 2003 , 3, 221-237	3.5	75
141	Lithium-Sulfur Batteries: State of the Art and Future Directions. <i>ACS Applied Energy Materials</i> , 2018 , 1, 1783-1814	6.1	74
140	Multiple steady states in reactive distillation: kinetic effects. <i>Computers and Chemical Engineering</i> , 2002 , 26, 81-93	4	72
139	Feasibility and separation sequencing in multicomponent batch distillation. <i>Chemical Engineering Science</i> , 1991 , 46, 1311-1326	4.4	72
138	Design and minimum-reflux calculations for double-feed multicomponent reactive distillation columns. <i>Chemical Engineering Science</i> , 1988 , 43, 2377-2389	4.4	68
137	A Novel Distillate Policy for Batch Reactive Distillation with Application to the Production of Butyl Acetate. <i>Industrial & Engineering Chemistry Research</i> , 1999 , 38, 714-722	3.9	66

136	Calculation of residue curve maps for mixtures with multiple equilibrium chemical reactions. <i>Industrial & Engineering Chemistry Research</i> , 1995 , 34, 3195-3202	3.9	66
135	Faceted crystal shape evolution during dissolution or growth. <i>AIChE Journal</i> , 2007 , 53, 1337-1348	3.6	65
134	Design and synthesis of heterogeneous azeotropic distillationsII. Column sequences. <i>Chemical Engineering Science</i> , 1990 , 45, 1845-1854	4.4	65
133	The interface between design and control. 1. Process controllability. <i>Industrial & Engineering Chemistry Research</i> , 1988 , 27, 597-605	3.9	64
132	Needle-Shaped Crystals: Causality and Solvent Selection Guidance Based on Periodic Bond Chains. <i>Crystal Growth and Design</i> , 2013 , 13, 3341-3352	3.5	63
131	Predictive Modeling of Supersaturation-Dependent Crystal Shapes. <i>Crystal Growth and Design</i> , 2012 , 12, 656-669	3.5	63
130	Design and synthesis of heterogeneous azeotropic distillationsII. Residue curve maps. <i>Chemical Engineering Science</i> , 1990 , 45, 1837-1843	4.4	63
129	Theory of phase equilibria in multireaction systems. <i>Chemical Engineering Science</i> , 1995 , 50, 3201-3216	4.4	62
128	Optimal design and synthesis of homogeneous azeotropic distillation sequences. <i>Industrial & Engineering Chemistry Research</i> , 1989 , 28, 564-572	3.9	61
127	Spiral Growth Model for Faceted Crystals of Non-Centrosymmetric Organic Molecules Grown from Solution. <i>Crystal Growth and Design</i> , 2011 , 11, 2780-2802	3.5	59
126	Predicting crystal growth by spiral motion. <i>Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences</i> , 2009 , 465, 1145-1171	2.4	58
125	Reactive distillation for methyl acetate production. <i>Computers and Chemical Engineering</i> , 2003 , 27, 1855-1866	4.866	57
124	Choosing an operating policy for seeded batch crystallization. <i>AIChE Journal</i> , 2006 , 52, 2046-2054	3.6	56
123	Design and synthesis of heterogeneous azeotropic distillationsII Heterogeneous phase diagrams. <i>Chemical Engineering Science</i> , 1990 , 45, 1823-1836	4.4	56
122	Patterns of composition change in multicomponent batch distillation. <i>Chemical Engineering Science</i> , 1990 , 45, 1207-1221	4.4	55
121	Size-Dependent Surface Free Energy and Tolman-Corrected Droplet Nucleation of TIP4P/2005 Water. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 4267-72	6.4	54
120	Simulation of kinetic effects in reactive distillation. <i>Computers and Chemical Engineering</i> , 2000 , 24, 2457-2472	4.472	53
119	Modeling of reactive distillation systems. <i>Industrial & Engineering Chemistry Research</i> , 1987 , 26, 983-989	3.99	50

118	Thermodynamic behavior of reactive azeotropes. <i>AIChE Journal</i> , 1997 , 43, 2227-2238	3.6	49
117	Green chemical engineering aspects of reactive distillation. <i>Environmental Science & Technology</i> , 2003 , 37, 5325-9	10.3	48
116	Design of three-component kinetically controlled reactive distillation columns using fixed-points methods. <i>Chemical Engineering Science</i> , 1994 , 49, 1947-1963	4.4	48
115	A design aid for crystal growth engineering. <i>Progress in Materials Science</i> , 2016 , 82, 1-38	42.2	48
114	Design of reactive extraction systems for bioproduct recovery. <i>AIChE Journal</i> , 2002 , 48, 514-526	3.6	47
113	Dynamics of heterogeneous azeotropic distillation columns. <i>AIChE Journal</i> , 1990 , 36, 39-52	3.6	47
112	Simultaneous prediction of crystal shape and size for solution crystallization. <i>AIChE Journal</i> , 2004 , 50, 2101-2112	3.6	46
111	Modeling the Crystal Shape of Polar Organic Materials: Prediction of Urea Crystals Grown from Polar and Nonpolar Solvents. <i>Crystal Growth and Design</i> , 2001 , 1, 455-461	3.5	46
110	Bifurcation study of kinetic effects in reactive distillation. <i>AIChE Journal</i> , 1999 , 45, 546-556	3.6	46
109	Communication: Bubbles, crystals, and laser-induced nucleation. <i>Journal of Chemical Physics</i> , 2011 , 134, 171102	3.9	45
108	Design/optimization of ternary heterogeneous azeotropic distillation sequences. <i>AIChE Journal</i> , 1989 , 35, 1592-1601	3.6	45
107	Reducing the mean size of API crystals by continuous manufacturing with product classification and recycle. <i>Chemical Engineering Science</i> , 2010 , 65, 5770-5780	4.4	44
106	A New Model for the Effect of Molecular Imposters on the Shape of Faceted Molecular Crystals. <i>Crystal Growth and Design</i> , 2009 , 9, 2637-2645	3.5	43
105	Necessary and sufficient conditions for reactive azeotropes in multireaction mixtures. <i>AIChE Journal</i> , 1995 , 41, 2383-2392	3.6	42
104	Calculation of solid-liquid equilibrium and crystallization paths for melt crystallization processes. <i>Chemical Engineering Science</i> , 1995 , 50, 1679-1694	4.4	41
103	The interface between design and control. 3. Selecting a set of controlled variables. <i>Industrial & Engineering Chemistry Research</i> , 1988 , 27, 611-615	3.9	40
102	Predicting the Effect of Solvent on the Crystal Habit of Small Organic Molecules. <i>Crystal Growth and Design</i> , 2016 , 16, 2590-2604	3.5	39
101	Crystal shape modification through cycles of dissolution and growth: Attainable regions and experimental validation. <i>AIChE Journal</i> , 2012 , 58, 1465-1474	3.6	39

100	The Evolution of Crystal Shape During Dissolution: Predictions and Experiments. <i>Crystal Growth and Design</i> , 2008 , 8, 1100-1101	3.5	39
99	Effect of Structurally Similar Additives on Crystal Habit of Organic Molecular Crystals at Low Supersaturation. <i>Crystal Growth and Design</i> , 2013 , 13, 1412-1428	3.5	38
98	Ion dissolution mechanism and kinetics at kink sites on NaCl surfaces. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, 656-661	11.5	37
97	Relative gain array for units in plants with recycle. <i>Industrial & Engineering Chemistry Research</i> , 1987 , 26, 1259-1262	3.9	37
96	Evolution of Crystal Shape. <i>Crystal Growth and Design</i> , 2004 , 4, 109-112	3.5	36
95	Separation of closely boiling mixtures by reactive distillation. 1. Theory. <i>Industrial & Engineering Chemistry Process Design and Development</i> , 1985 , 24, 1062-1071		36
94	A dynamic model for evolution of crystal shape. <i>Journal of Crystal Growth</i> , 2004 , 267, 239-250	1.6	35
93	Predicting the shape of organic crystals grown from polar solvents. <i>Chemical Engineering Science</i> , 2002 , 57, 1805-1813	4.4	35
92	On the dynamics of distillation processesVI. batch distillation. <i>Chemical Engineering Science</i> , 1985 , 40, 2087-2093	4.4	34
91	Feasible region for a countercurrent cascade of vapor-liquid CSTRs. <i>AIChE Journal</i> , 2002 , 48, 800-814	3.6	33
90	Design for Simultaneous Reaction and Liquid-Liquid Extraction. <i>Industrial & Engineering Chemistry Research</i> , 1998 , 37, 4748-4755	3.9	33
89	Geometric nonlinear analysis of multicomponent nonideal distillation: a simple computer-aided design procedure. <i>Chemical Engineering Science</i> , 1993 , 48, 1367-1391	4.4	33
88	Design and minimum reflux for heterogeneous azeotropic distillation columns. <i>AIChE Journal</i> , 1989 , 35, 1585-1591	3.6	32
87	Effect of chemical kinetics on feasible splits for reactive distillation. <i>AIChE Journal</i> , 2001 , 47, 590-601	3.6	31
86	The interface between design and control. 2. Process operability. <i>Industrial & Engineering Chemistry Research</i> , 1988 , 27, 606-611	3.9	31
85	Design and synthesis of homogeneous azeotropic distillations. 4. Minimum reflux calculations for multiple-feed columns. <i>Industrial & Engineering Chemistry Fundamentals</i> , 1986 , 25, 269-279		31
84	Manipulation of crystal shape by cycles of growth and dissolution. <i>AIChE Journal</i> , 2007 , 53, 1510-1517	3.6	30
83	Natural gas conversion to liquid fuels in a zone reactor. <i>Catalysis Today</i> , 2005 , 106, 301-304	5.3	30

82	A simulation test of the optical Kerr mechanism for laser-induced nucleation. <i>Journal of Chemical Physics</i> , 2011 , 134, 154501	3.9	29
81	Rate Expressions for Kink Attachment and Detachment During Crystal Growth. <i>Crystal Growth and Design</i> , 2016 , 16, 3313-3322	3.5	28
80	Separation of conglomerate forming enantiomers using a novel continuous preferential crystallization process. <i>AIChE Journal</i> , 2015 , 61, 2810-2823	3.6	27
79	Estimating diffusivity along a reaction coordinate in the high friction limit: Insights on pulse times in laser-induced nucleation. <i>Journal of Chemical Physics</i> , 2009 , 131, 224112	3.9	26
78	A Geometric Design Method for Side-Stream Distillation Columns. <i>Industrial & Engineering Chemistry Research</i> , 1996 , 35, 3653-3664	3.9	26
77	On the dynamics of distillation processes-V. <i>Chemical Engineering Science</i> , 1984 , 39, 883-892	4.4	26
76	Modeling layered crystal growth at increasing supersaturation by connecting growth regimes. <i>AIChE Journal</i> , 2017 , 63, 1338-1352	3.6	24
75	Steady State Morphologies of Paracetamol Crystal from Different Solvents. <i>Crystal Growth and Design</i> , 2017 , 17, 659-670	3.5	24
74	Material stability of multicomponent mixtures and the multiplicity of solutions to phase-equilibrium equations. 1. Nonreacting mixtures. <i>Industrial & Engineering Chemistry Fundamentals</i> , 1983 , 22, 472-485		24
73	Nucleation and polymorph selection in a model colloidal fluid. <i>Physical Review E</i> , 2008 , 77, 041604	2.4	23
72	A systematic method for reaction invariants and mole balances for complex chemistries. <i>Computers and Chemical Engineering</i> , 2001 , 25, 1199-1217	4	23
71	A simple exact method for calculating tangent pinch points in multicomponent nonideal mixtures by bifurcation theory. <i>Chemical Engineering Science</i> , 1986 , 41, 3155-3160	4.4	23
70	Designing Robust Crystallization Processes in the Presence of Parameter Uncertainty Using Attainable Regions. <i>Industrial & Engineering Chemistry Research</i> , 2015 , 54, 10350-10363	3.9	22
69	Feasible products for kinetically controlled reactive distillation of ternary mixtures. <i>AIChE Journal</i> , 2000 , 46, 923-936	3.6	22
68	A Geometric Method for the Design of Liquid Extractors. <i>Industrial & Engineering Chemistry Research</i> , 1996 , 35, 2672-2681	3.9	22
67	The presynthesis problem for homogeneous azeotropic distillation has a unique explicit solution. <i>Chemical Engineering Science</i> , 1985 , 40, 1885-1889	4.4	22
66	Design and synthesis of homogeneous azeotropic distillations. 5. Columns with nonnegligible heat effects. <i>Industrial & Engineering Chemistry Fundamentals</i> , 1986 , 25, 279-289		22
65	Screening of process retrofit alternatives. <i>Industrial & Engineering Chemistry Research</i> , 1987 , 26, 2195-2204	3.9	21

64	Separation of closely boiling mixtures by reactive distillation. 2. Experiments. <i>Industrial & Engineering Chemistry Process Design and Development</i> , 1985 , 24, 1071-1073		21
63	Modeling Olanzapine Solution Growth Morphologies. <i>Crystal Growth and Design</i> , 2018 , 18, 905-911	3.5	21
62	Importance of Process Chemistry in Selecting the Operating Policy for Plants with Recycle□ <i>Industrial & Engineering Chemistry Research</i> , 2004 , 43, 3957-3971	3.9	20
61	Computing All Homogeneous and Heterogeneous Azeotropes in Multicomponent Mixtures. <i>Industrial & Engineering Chemistry Research</i> , 1999 , 38, 4901-4912	3.9	20
60	Energetic and entropic components of the Tolman length for mW and TIP4P/2005 water nanodroplets. <i>Journal of Chemical Physics</i> , 2016 , 145, 204703	3.9	20
59	Approximate dynamic models for chemical process systems. <i>Industrial & Engineering Chemistry Research</i> , 1989 , 28, 546-552	3.9	19
58	Synthesis of Azeotropic Distillation Systems with Recycles. <i>Industrial & Engineering Chemistry Research</i> , 2003 , 42, 1783-1794	3.9	18
57	Polymorph selection by continuous crystallization. <i>AIChE Journal</i> , 2016 , 62, 3505-3514	3.6	18
56	A mechanistic growth model for inorganic crystals: Growth mechanism. <i>AIChE Journal</i> , 2014 , 60, 3720-3736	3.6	17
55	A new framework and a simpler method for the development of batch crystallization recipes. <i>AIChE Journal</i> , 2011 , 57, 606-617	3.6	17
54	Selectivity Targets for Batch Reactive Distillation□ <i>Industrial & Engineering Chemistry Research</i> , 2000 , 39, 1565-1575	3.9	17
53	Kink Rate Model for the General Case of Organic Molecular Crystals. <i>Crystal Growth and Design</i> , 2014 , 14, 2460-2467	3.5	16
52	Materials science. Imaging crystallization. <i>Science</i> , 2014 , 344, 705-6	33.3	15
51	Multisite models to determine the distribution of kink sites adjacent to low-energy edges. <i>Physical Review E</i> , 2012 , 85, 021604	2.4	15
50	A stochastic model for the critical length of a spiral edge. <i>Journal of Crystal Growth</i> , 2010 , 312, 785-792	1.6	15
49	Insight from Economically Optimal Steady-State Operating Policies for Dynamic Plantwide Control. <i>Industrial & Engineering Chemistry Research</i> , 2006 , 45, 1343-1353	3.9	15
48	Plantwide dynamics and control of processes with crystallization. <i>Computers and Chemical Engineering</i> , 2010 , 34, 112-121	4	14
47	Feasibility and synthesis of hybrid reactive distillation systems. <i>AIChE Journal</i> , 2002 , 48, 2754-2768	3.6	14

46	Design and operating targets for nonideal multicomponent batch distillation. <i>Industrial & Engineering Chemistry Research</i> , 1993 , 32, 293-301	3.9	14
45	Wiped film reactor model for nylon 6,6 polymerization. <i>Industrial & Engineering Chemistry Research</i> , 1990 , 29, 2012-2020	3.9	14
44	Target bounds on reaction selectivity via Feinberg's CFSTR equivalence principle. <i>AIChE Journal</i> , 2018 , 64, 926-939	3.6	13
43	Reinterpreting edge energies calculated from crystal growth experiments. <i>Journal of Crystal Growth</i> , 2011 , 327, 117-126	1.6	13
42	Plantwide operation of processes with crystallization. <i>AIChE Journal</i> , 2007 , 53, 2885-2896	3.6	13
41	Simultaneous kinetic resolution of chiral propylene oxide and propylene glycol in a continuous reactive distillation column. <i>Chemical Engineering Science</i> , 2003 , 58, 1289-1300	4.4	13
40	Controlling thermally linked distillation columns. <i>Industrial & Engineering Chemistry Process Design and Development</i> , 1984 , 23, 483-490		13
39	A mechanistic growth model for inorganic crystals: Solid-state interactions. <i>AIChE Journal</i> , 2014 , 60, 3707-3719	3.7	12
38	Crystallization of selective polymorph using relationship between supersaturation and solubility. <i>AIChE Journal</i> , 2015 , 61, 1372-1379	3.6	12
37	Effect of Competing Reversible Reactions on Optimal Operating Policies for Plants with Recycle. <i>Industrial & Engineering Chemistry Research</i> , 2009 , 48, 8037-8047	3.9	12
36	An approximate model for binary azeotropic distillation design. <i>Chemical Engineering Science</i> , 1984 , 39, 11-19	4.4	12
35	In Silico Crystal Growth Rate Prediction for NaCl from Aqueous Solution. <i>Crystal Growth and Design</i> , 2018 , 18, 6302-6306	3.5	12
34	Modeling Step Velocities and Edge Surface Structures during Growth of Non-Centrosymmetric Crystals. <i>Crystal Growth and Design</i> , 2017 , 17, 2066-2080	3.5	11
33	Properties of liquid-vapour composition surfaces for multicomponent mixtures with constant latent heat. <i>Chemical Engineering Science</i> , 1985 , 40, 1979-1980	4.4	11
32	Polymorph Selection by Continuous Precipitation. <i>Crystal Growth and Design</i> , 2018 , 18, 4306-4319	3.5	10
31	Novel Reactor Temperature and Recycle Flow Rate Policies for Optimal Process Operation in the Plantwide Context. <i>Industrial & Engineering Chemistry Research</i> , 2005 , 44, 6729-6740	3.9	10
30	New tools for the design of kinetically controlled reactive distillation columns. <i>Computers and Chemical Engineering</i> , 1994 , 18, S1-S13	4	10
29	Effect of overdesign on the operability of distillation columns. <i>Industrial & Engineering Chemistry Process Design and Development</i> , 1985 , 24, 593-598		10

28	Reaction Invariants and Mole Balances for Plant Complexes. <i>Industrial & Engineering Chemistry Research</i> , 2002 , 41, 3771-3783	3.9	9
27	New Tricks of the Trade for Crystal Structure Refinement. <i>ACS Central Science</i> , 2017 , 3, 726-733	16.8	8
26	Thermodynamic assessment of carbon dioxide emission reduction during fossil fuel derived energy production. <i>Energy</i> , 2019 , 177, 565-573	7.9	8
25	Reformulating multidimensional population balances for predicting crystal size and shape. <i>AICHE Journal</i> , 2013 , 59, 3468-3474	3.6	8
24	Feasible Regions for Step-Growth Melt Polycondensation Systems. <i>Industrial & Engineering Chemistry Research</i> , 2004 , 43, 428-440	3.9	8
23	Selection of reference components in reaction invariants. <i>Chemical Engineering Science</i> , 2005 , 60, 7168-7171	4.1	7
22	Feasible Products for Double-Feed Reactive Distillation Columns. <i>Industrial & Engineering Chemistry Research</i> , 2007 , 46, 3255-3264	3.9	6
21	Ultimate bounds on reaction selectivity for batch reactors. <i>Chemical Engineering Science</i> , 2019 , 199, 652-660	4.4	6
20	Performing solvation free energy calculations in LAMMPS using the decoupling approach. <i>Journal of Computer-Aided Molecular Design</i> , 2020 , 34, 641-646	4.2	5
19	A New Software Framework for Implementing Crystal Growth Models to Materials of Any Crystallographic Complexity. <i>Crystal Growth and Design</i> , 2020 , 20, 2885-2892	3.5	4
18	A tribute to professor Roger Sargent: Intellectual leader of process systems engineering. <i>AICHE Journal</i> , 2016 , 62, 2951-2958	3.6	4
17	Analytical Design and Operation of Systems with Crystallization, Filtration, and Recycling. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 1196-1205	3.9	4
16	Steady-State Operating Policies for Plants with Multiple Reactions of Equal Overall Order. <i>Industrial & Engineering Chemistry Research</i> , 2006 , 45, 8056-8062	3.9	4
15	Digital design of crystalline solids. <i>Computers and Chemical Engineering</i> , 2020 , 133, 106637	4	4
14	Critical length of a one-dimensional nucleus. <i>Journal of Chemical Physics</i> , 2016 , 145, 211916	3.9	4
13	Ultimate Reaction Selectivity Limits for Intensified Reactor-Separators. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 6042-6048	3.9	4
12	Nonequilibrium Kink Density from One-Dimensional Nucleation for Step Velocity Predictions. <i>Crystal Growth and Design</i> , 2018 , 18, 723-727	3.5	3
11	Attainable Regions in Crystallization Processes. <i>Computer Aided Chemical Engineering</i> , 2014 , 34, 465-470	3.6	3

10	Selectivity versus conversion and optimal operating policies for plants with recycle. <i>AICHE Journal</i> , 2008 , 54, 2597-2609	3.6	3
9	Effects of vapor-liquid mass transfer on feasibility of reactive distillation. <i>AICHE Journal</i> , 2004 , 50, 1795-1813	3.6	2
8	Experimental study of feasibility in kinetically-controlled reactive distillation. <i>AICHE Journal</i> , 2005 , 51, 464-479	3.6	2
7	A rapid screening methodology for chemical processes. <i>Computers and Chemical Engineering</i> , 2020 , 142, 107039	4	2
6	Free energies of crystals computed using Einstein crystal with fixed center of mass and differing spring constants. <i>Journal of Chemical Physics</i> , 2021 , 154, 164509	3.9	2
5	Distillation, Azeotropic, and Extractive 2004 ,		1
4	Absolute chemical potentials for complex molecules in fluid phases: A centroid reference for predicting phase equilibria. <i>Journal of Chemical Physics</i> , 2020 , 153, 214504	3.9	0
3	Innovation in Chemical Reactor Engineering Practice and Science. <i>Computers and Chemical Engineering</i> , 2022 , 107699	4	
2	Ultimate Reaction Selectivities and Screening-Level Metrics for Conceptual Design. <i>Computer Aided Chemical Engineering</i> , 2019 , 329-334	0.6	
1	Crystal Morphology Modeling of Solvates and Hydrates of Organic Molecular Crystals: Olanzapine Solvate and Dihydrate. <i>Crystal Growth and Design</i> , 2021 , 21, 4871-4877	3.5	