

Chau-Chyun Chen

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127
papers

6,289
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136
ext. papers

6,945
ext. citations

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avg, IF

6.04
L-index

#	Paper	IF	Citations
127	Local composition model for excess Gibbs energy of electrolyte systems. Part I: Single solvent, single completely dissociated electrolyte systems. <i>AIChE Journal</i> , 1982 , 28, 588-596	3.6	707
126	A local composition model for the excess Gibbs energy of aqueous electrolyte systems. <i>AIChE Journal</i> , 1986 , 32, 444-454	3.6	704
125	Model of vapor-liquid equilibria for aqueous acid gas-alkanolamine systems using the electrolyte-NRTL equation. <i>Industrial & Engineering Chemistry Research</i> , 1989 , 28, 1060-1073	3.9	406
124	Thermodynamic representation of phase equilibria of mixed-solvent electrolyte systems. <i>AIChE Journal</i> , 1986 , 32, 1655-1664	3.6	307
123	Model of vapor-liquid equilibria for aqueous acid gas-alkanolamine systems. 2. Representation of hydrogen sulfide and carbon dioxide solubility in aqueous MDEA and carbon dioxide solubility in aqueous mixtures of MDEA with MEA or DEA. <i>Industrial & Engineering Chemistry Research</i> , 1991 , 30, 543-555	3.9	249
122	Sigma-Profile Database for Using COSMO-Based Thermodynamic Methods. <i>Industrial & Engineering Chemistry Research</i> , 2006 , 45, 4389-4415	3.9	238
121	Rate-Based Process Modeling Study of CO ₂ Capture with Aqueous Monoethanolamine Solution. <i>Industrial & Engineering Chemistry Research</i> , 2009 , 48, 9233-9246	3.9	205
120	Generalized electrolyte-NRTL model for mixed-solvent electrolyte systems. <i>AIChE Journal</i> , 2004 , 50, 1928-1941	3.6	185
119	Solubility Modeling with a Nonrandom Two-Liquid Segment Activity Coefficient Model. <i>Industrial & Engineering Chemistry Research</i> , 2004 , 43, 8354-8362	3.9	165
118	A segment-based local composition model for the gibbs energy of polymer solutions. <i>Fluid Phase Equilibria</i> , 1993 , 83, 301-312	2.5	154
117	Refinement of COSMOBAC and the Applications. <i>Industrial & Engineering Chemistry Research</i> , 2007 , 46, 7275-7288	3.9	148
116	Symmetric Electrolyte Nonrandom Two-Liquid Activity Coefficient Model. <i>Industrial & Engineering Chemistry Research</i> , 2009 , 48, 7788-7797	3.9	147
115	Extension and application of the pitzer equation for vapor-liquid equilibrium of aqueous electrolyte systems with molecular solutes. <i>AIChE Journal</i> , 1979 , 25, 820-831	3.6	133
114	Correlation and Prediction of Drug Molecule Solubility in Mixed Solvent Systems with the Nonrandom Two-Liquid Segment Activity Coefficient (NRTL _{BAC}) Model. <i>Industrial & Engineering Chemistry Research</i> , 2006 , 45, 4816-4824	3.9	129
113	Thermodynamic Modeling for CO ₂ Absorption in Aqueous MDEA Solution with Electrolyte NRTL Model. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 163-175	3.9	125
112	Applied thermodynamics for process modeling. <i>AIChE Journal</i> , 2002 , 48, 194-200	3.6	125
111	Thermodynamic modeling for CO ₂ absorption in aqueous MEA solution with electrolyte NRTL model. <i>Fluid Phase Equilibria</i> , 2011 , 311, 67-75	2.5	115

110	Phase Partitioning of Biomolecules: Solubilities of Amino Acids. <i>Biotechnology Progress</i> , 1989 , 5, 111-118	2.8	100
109	New mass-transfer correlations for packed towers. <i>AIChE Journal</i> , 2012 , 58, 132-152	3.6	88
108	Modeling CO ₂ Absorption and Desorption by Aqueous Monoethanolamine Solution with Aspen Rate-based Model. <i>Energy Procedia</i> , 2013 , 37, 1584-1596	2.3	75
107	Prediction of pharmaceutical solubility Via NRTL-SAC and COSMO-SAC. <i>Journal of Pharmaceutical Sciences</i> , 2008 , 97, 1813-20	3.9	72
106	Use of hydration and dissociation chemistries with the electrolyte-NRTL model. <i>AIChE Journal</i> , 1999 , 45, 1576-1586	3.6	72
105	Steady-State and Dynamic Modeling of Commercial Slurry High-Density Polyethylene (HDPE) Processes. <i>Industrial & Engineering Chemistry Research</i> , 2002 , 41, 5601-5618	3.9	68
104	Thermodynamic Modeling of the NH ₃ /CO ₂ /H ₂ O System with Electrolyte NRTL Model. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 11406-11421	3.9	64
103	Refined electrolyte-NRTL model: Activity coefficient expressions for application to multi-electrolyte systems. <i>AIChE Journal</i> , 2008 , 54, 1608-1624	3.6	61
102	Steady-State and Dynamic Modeling of Gas-Phase Polypropylene Processes Using Stirred-Bed Reactors. <i>Industrial & Engineering Chemistry Research</i> , 2004 , 43, 884-900	3.9	60
101	Thermodynamic modeling of CO ₂ and H ₂ S solubilities in aqueous DIPA solution, aqueous sulfolane/DIPA solution, and aqueous sulfolane/DEA solution with electrolyte NRTL model. <i>Fluid Phase Equilibria</i> , 2011 , 306, 190-203	2.5	56
100	Thermodynamic modeling of CO ₂ solubility in aqueous solutions of NaCl and Na ₂ SO ₄ . <i>Journal of Supercritical Fluids</i> , 2010 , 55, 623-634	4.2	47
99	Liquid Viscosity Model for Polymer Solutions and Mixtures. <i>Industrial & Engineering Chemistry Research</i> , 2003 , 42, 2415-2422	3.9	44
98	Thermodynamic Modeling of the Sulfuric Acid/Water/Sulfur Trioxide System with the Symmetric Electrolyte NRTL Model. <i>Journal of Chemical & Engineering Data</i> , 2011 , 56, 963-977	2.8	43
97	Segment-Based Eyring-NRTL Viscosity Model for Mixtures Containing Polymers. <i>Industrial & Engineering Chemistry Research</i> , 2004 , 43, 6231-6237	3.9	43
96	Equation of State Modeling of Phase Equilibrium in the Low-Density Polyethylene Process: The Sanchez-Lacombe, Statistical Associating Fluid Theory, and Polymer-Soave-Redlich-Kwong Equations of State. <i>Industrial & Engineering Chemistry Research</i> , 1998 , 37, 4481-4491	3.9	43
95	Fragment-Based Approach for Estimating Thermophysical Properties of Fats and Vegetable Oils for Modeling Biodiesel Production Processes. <i>Industrial & Engineering Chemistry Research</i> , 2010 , 49, 876-886	3.9	42
94	Thermodynamic representation of the NaCl+Na ₂ SO ₄ +H ₂ O system with electrolyte NRTL model. <i>Fluid Phase Equilibria</i> , 2011 , 306, 149-161	2.5	36
93	Correlation and Prediction of Phase Behavior of Organic Compounds in Ionic Liquids Using the Nonrandom Two-Liquid Segment Activity Coefficient Model. <i>Industrial & Engineering Chemistry Research</i> , 2008 , 47, 7081-7093	3.9	36

92	Quantifying Relationships among the Molecular Weight Distribution, Non-Newtonian Shear Viscosity, and Melt Index for Linear Polymers. <i>Industrial & Engineering Chemistry Research</i> , 2003 , 42, 5354-5362	3.9	36
91	Modeling Polyethylene Fractionation Using the Perturbed-Chain Statistical Associating Fluid Theory Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2002 , 41, 968-988	3.9	33
90	Segment-based excess Gibbs energy model for aqueous organic electrolytes. <i>AIChE Journal</i> , 2001 , 47, 2593-2602	3.6	32
89	Toward development of activity coefficient models for process and product design of complex chemical systems. <i>Fluid Phase Equilibria</i> , 2006 , 241, 103-112	2.5	31
88	Representation of solid-liquid equilibrium of aqueous electrolyte systems with the electrolyte NRTL model. <i>Fluid Phase Equilibria</i> , 1986 , 27, 457-474	2.5	31
87	Extension of Nonrandom Two-Liquid Segment Activity Coefficient Model for Electrolytes. <i>Industrial & Engineering Chemistry Research</i> , 2005 , 44, 8909-8921	3.9	27
86	Thermodynamic modeling of KCl + H ₂ O and KCl + NaCl + H ₂ O systems using electrolyte NRTL model. <i>Fluid Phase Equilibria</i> , 2015 , 387, 169-177	2.5	26
85	Polymer-Solvent Vapor-Liquid Equilibrium: Equations of State versus Activity Coefficient Models. <i>Industrial & Engineering Chemistry Research</i> , 1998 , 37, 1567-1573	3.9	26
84	Molecular thermodynamic model for gibbs energy of mixing of nonionic surfactant solutions. <i>AIChE Journal</i> , 1996 , 42, 3231-3240	3.6	26
83	Modeling Drug Molecule Solubility to Identify Optimal Solvent Systems for Crystallization. <i>Organic Process Research and Development</i> , 2008 , 12, 249-256	3.9	25
82	Thermodynamic modeling of aqueous Ca ²⁺ -Na ⁺ -K ⁺ -Cl ⁻ quaternary system. <i>Fluid Phase Equilibria</i> , 2016 , 409, 193-206	2.5	24
81	An extension of cubic equations of state to vapor-liquid equilibria in polymer-solvent mixtures. <i>Fluid Phase Equilibria</i> , 1998 , 145, 169-192	2.5	24
80	A New Phase-Equilibrium Model for Simulating Industrial Nylon-6 Production Trains. <i>Industrial & Engineering Chemistry Research</i> , 2003 , 42, 3900-3913	3.9	24
79	Predicting Thermophysical Properties of Mono- and Diglycerides with the Chemical Constituent Fragment Approach. <i>Industrial & Engineering Chemistry Research</i> , 2010 , 49, 5479-5484	3.9	22
78	COSMO-SAC Sigma Profile Generation with Conceptual Segment Concept. <i>Industrial & Engineering Chemistry Research</i> , 2015 , 54, 4441-4454	3.9	21
77	Optimal Solvent Screening for the Crystallization of Pharmaceutical Compounds from Multisolvent Systems. <i>Industrial & Engineering Chemistry Research</i> , 2012 , 51, 13792-13802	3.9	21
76	Microfluidic production of size-tunable hexadecane-in-water emulsions: Effect of droplet size on destabilization of two-dimensional emulsions due to partial coalescence. <i>Journal of Colloid and Interface Science</i> , 2019 , 533, 59-70	9.3	20
75	Extension of COSMO-SAC Solvation Model for Electrolytes. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 176-187	3.9	20

74	Predicting NRTL binary interaction parameters from molecular simulations. <i>AIChE Journal</i> , 2018 , 64, 2758-2769	3.6	19
73	Temperature dependence of interaction parameters in electrolyte NRTL model. <i>AIChE Journal</i> , 2016 , 62, 1244-1253	3.6	19
72	Modeling Gas Solubilities in the Aqueous Solution of Methyl-diethanolamine. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 6436-6446	3.9	19
71	Use of GAMESS/COSMO program in support of COSMO-SAC model applications in phase equilibrium prediction calculations. <i>Fluid Phase Equilibria</i> , 2009 , 276, 37-45	2.5	17
70	A molecular thermodynamic approach to predict the secondary structure of homopolypeptides in aqueous systems. <i>Biopolymers</i> , 1992 , 32, 1375-92	2.2	17
69	Thermodynamic model of aqueous Mg ²⁺ - Na ⁺ - K ⁺ - Cl ⁻ quaternary system. <i>Fluid Phase Equilibria</i> , 2017 , 437, 56-68	2.5	16
68	A segment contribution method for the vapor pressure of tall-oil chemicals. <i>Fluid Phase Equilibria</i> , 1999 , 155, 193-203	2.5	16
67	Comprehensive thermodynamic modeling of saline water with electrolyte NRTL model: A study on aqueous Ba ²⁺ - Na ⁺ - Cl ⁻ - SO ₄ ²⁻ quaternary system. <i>Fluid Phase Equilibria</i> , 2017 , 447, 29-38	2.5	15
66	New Mass-Transfer Model for Simulating Industrial Nylon-6 Production Trains. <i>Industrial & Engineering Chemistry Research</i> , 2004 , 43, 5063-5076	3.9	15
65	Representation of phase equilibrium behavior of antibiotics. <i>Biotechnology Progress</i> , 1990 , 6, 266-72	2.8	15
64	Thermodynamic modeling of aqueous Na ⁺ - K ⁺ - Cl ⁻ - SO ₄ ²⁻ quaternary system with electrolyte NRTL model. <i>Fluid Phase Equilibria</i> , 2015 , 403, 1-9	2.5	14
63	Multicomponent flash algorithm for mixtures containing polydisperse polymers. <i>AIChE Journal</i> , 2003 , 49, 258-268	3.6	14
62	Revisiting electrolyte thermodynamic models: Insights from molecular simulations. <i>AIChE Journal</i> , 2018 , 64, 3728-3734	3.6	13
61	Local composition activity coefficient model for mixed-gas adsorption equilibria. <i>Adsorption</i> , 2019 , 25, 951-964	2.6	12
60	Symmetric Nonrandom Two-Liquid Segment Activity Coefficient Model for Electrolytes. <i>Industrial & Engineering Chemistry Research</i> , 2009 , 48, 5522-5529	3.9	12
59	Comprehensive thermodynamic modeling of saline water with electrolyte NRTL model: A study of aqueous Sr ²⁺ - Na ⁺ - Cl ⁻ - SO ₄ ²⁻ quaternary system. <i>Fluid Phase Equilibria</i> , 2018 , 470, 221-231	2.5	12
58	Thermodynamic representation of aqueous sodium nitrate and nitric acid solution with electrolyte NRTL model. <i>Fluid Phase Equilibria</i> , 2016 , 407, 105-116	2.5	11
57	Nonrandom Two-Liquid Segment Activity Coefficient Model with Association Theory. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 12773-12786	3.9	11

56	Aggregation thermodynamics for asphaltene precipitation. <i>AIChE Journal</i> , 2016 , 62, 1254-1264	3.6	11
55	Development of a Thermophysical Properties Model for Flowsheet Simulation of Biomass Pyrolysis Processes. <i>ACS Sustainable Chemistry and Engineering</i> , 2019 , 7, 9017-9027	8.3	10
54	A comprehensive thermodynamic model for high salinity produced waters. <i>AIChE Journal</i> , 2020 , 66, e16818	3.8	10
53	Bridging two-liquid theory with molecular simulations for electrolytes: An investigation of aqueous NaCl solution. <i>AIChE Journal</i> , 2019 , 65, 1315-1324	3.6	10
52	Melting Behavior and Heat of Fusion of Compounds that Undergo Simultaneous Melting and Decomposition: An investigation with HMX. <i>Journal of Chemical & Engineering Data</i> , 2017 , 62, 967-972	3.8	9
51	Nonrandom two-liquid activity coefficient model for aqueous polyelectrolyte solutions. <i>Fluid Phase Equilibria</i> , 2019 , 497, 1-9	2.5	9
50	Thermodynamic modeling of the hybrid sulfur (HyS) cycle for hydrogen production. <i>Fluid Phase Equilibria</i> , 2018 , 460, 175-188	2.5	9
49	An activity-based formulation for Langmuir adsorption isotherm. <i>Adsorption</i> , 2020 , 26, 375-386	2.6	9
48	Performance of sweeping gas membrane distillation for treating produced water: Modeling and experiments. <i>Desalination</i> , 2020 , 492, 114597	10.3	9
47	Nonrandom two-liquid activity coefficient model with association theory. <i>AIChE Journal</i> , 2021 , 67,	3.6	9
46	Mobile ion partitioning in ion exchange membranes immersed in saline solutions. <i>Journal of Membrane Science</i> , 2021 , 620, 118760	9.6	9
45	Thermodynamic modeling of HNO ₃ -H ₂ SO ₄ -H ₂ O ternary system with symmetric electrolyte NRTL model. <i>AIChE Journal</i> , 2017 , 63, 3110-3117	3.6	8
44	Thermodynamic modeling of aqueous Na ⁺ -K ⁺ -Mg ²⁺ -SO ₄ ²⁻ quaternary system. <i>Fluid Phase Equilibria</i> , 2015 , 404, 141-149	2.5	8
43	Thermodynamic modeling of asphaltene precipitation in pure and mixed solvents with NRTL-SAC. <i>Fluid Phase Equilibria</i> , 2018 , 473, 255-261	2.5	8
42	Thermodynamic modeling of HCl-H ₂ O binary system with symmetric electrolyte NRTL model. <i>Journal of Chemical Thermodynamics</i> , 2018 , 125, 159-171	2.9	8
41	Molecular thermodynamic modeling of aqueous Na ⁺ -K ⁺ -Mg ²⁺ -Ca ²⁺ -SO ₄ ²⁻ quinary system. <i>Fluid Phase Equilibria</i> , 2019 , 491, 77-87	2.5	7
40	Some recent developments in process simulation for reactive chemical systems. <i>Pure and Applied Chemistry</i> , 1987 , 59, 1177-1188	2.1	7
39	Prediction of Asphaltene Precipitation in Organic Solvents via COSMO-SAC. <i>Energy & Fuels</i> , 2017 , 31, 8985-8996	4.1	6

38	Modeling swelling behavior of hydrogels in aqueous organic solvents. <i>Chemical Engineering Science</i> , 2021 , 242, 116744	4.4	6
37	Correlation and prediction of drug molecule solubility with the NRTL-SAC model. <i>Computer Aided Chemical Engineering</i> , 2006 , 859-864	0.6	5
36	Molecular thermodynamic model to predict the alpha-helical secondary structure of polypeptide chains in solution. <i>Biochemistry</i> , 1992 , 31, 10591-601	3.2	5
35	Solubility of Nutraceutical Compounds in Generally Recognized as Safe Solvents at 298 K. <i>International Journal of Chemical Engineering and Applications (IJCEA)</i> , 2016 , 7, 289-294	0.2	5
34	A Novel Approach to Modeling Biomass Pyrolysis in a Fluidized Bed Reactor. <i>ACS Sustainable Chemistry and Engineering</i> , 2020 , 8, 14605-14615	8.3	5
33	Thermodynamic modeling of CO ₂ absorption in aqueous potassium carbonate solution with electrolyte NRTL model. <i>Fluid Phase Equilibria</i> , 2020 , 505, 112339	2.5	5
32	Isosteric heat of adsorption from thermodynamic Langmuir isotherm. <i>Adsorption</i> , 2021 , 27, 979-989	2.6	5
31	Association-based activity coefficient model for electrolyte solutions. <i>AIChE Journal</i> , e17422	3.6	4
30	Aggregation thermodynamics of asphaltenes: Prediction of asphaltene precipitation in petroleum fluids with NRTL-SAC. <i>Fluid Phase Equilibria</i> , 2020 , 520, 112655	2.5	3
29	Prediction of mixed-gas adsorption equilibria from pure component adsorption isotherms. <i>AIChE Journal</i> , 2020 , 66, e16243	3.6	3
28	Prediction of thermodynamic properties of organic mixtures: Combining molecular simulations with classical thermodynamics. <i>Fluid Phase Equilibria</i> , 2020 , 523, 112759	2.5	3
27	Thermodynamic Modeling of Aqueous LiCl, LiBr, LiI, and LiNO ₃ Solutions. <i>Fluid Phase Equilibria</i> , 2021 , 531, 112914	2.5	3
26	Modeling dissociation of ionic liquids with electrolyte NRTL model. <i>Journal of Molecular Liquids</i> , 2021 , 329, 115524	6	3
25	Prediction of χ Parameter of Polymer Blends by Combining Molecular Simulations and Integral Equation Theory. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 9022-9031	3.4	3
24	Molecular thermodynamics for scaling prediction: Case of membrane distillation. <i>Separation and Purification Technology</i> , 2021 , 276, 119231	8.3	3
23	Collective nucleation dynamics in two-dimensional emulsions with hexagonal packing. <i>Physical Review E</i> , 2020 , 101, 030602	2.4	2
22	Correlations for Densities of Aqueous Electrolyte Solutions. <i>Journal of Chemical & Engineering Data</i> , 2016 , 61, 740-747	2.8	2
21	Process simulation in polymer manufacturing. <i>Computers and Chemical Engineering</i> , 1992 , 16, S481-S490	4	2

20	The role of computerized modeling and simulation in the development of life support system technologies. <i>Advances in Space Research</i> , 1989 , 9, 121-31	2.4	2
19	Environmental Impacts of Hydraulic Fracturing 2016 , 199-219		2
18	Predicting wax appearance temperature and precipitation profile of normal alkane systems: An explicit co-crystal model. <i>Fluid Phase Equilibria</i> , 2020 , 509, 112466	2.5	2
17	A simple and practical process modeling methodology for pressure swing adsorption. <i>Computers and Chemical Engineering</i> , 2021 , 147, 107235	4	2
16	A rigorous process modeling methodology for biomass fast pyrolysis with an entrained-flow reactor. <i>Journal of Advanced Manufacturing and Processing</i> , 2020 , 2,	2.7	2
15	Modeling aqueous multivalent polyelectrolytes systems with polyelectrolyte NRTL model. <i>Journal of Molecular Liquids</i> , 2021 , 336, 116237	6	2
14	Solubility Thermodynamics of Organic Energetic Materials 2017 , 43-62		1
13	Modeling fluid phase equilibria of carbon dioxide-methanol binary system. <i>Fluid Phase Equilibria</i> , 2021 , 529, 112866	2.5	1
12	Modeling Phase Equilibrium of Common Sugars Glucose, Fructose, and Sucrose in Mixed Solvents. <i>Journal of Chemical & Engineering Data</i> ,	2.8	1
11	Extended thermodynamic model for high salinity produced waters. <i>Chemical Engineering Science</i> , 2021 , 243, 116754	4.4	1
10	Molecular Thermodynamics for Pharmaceutical Process Modeling and Simulation 505-519		1
9	Catastrophic thermal destabilization of two-dimensional close-packed emulsions due to synchronous coalescence initiation. <i>Soft Matter</i> , 2020 , 16, 6032-6037	3.6	0
8	From Langmuir isotherm to Brunauer-Emmett-Teller isotherm. <i>AIChE Journal</i> , e17523	3.6	0
7	Thermodynamic analysis of hydrogel swelling in aqueous sodium chloride solutions. <i>Journal of Molecular Liquids</i> , 2022 , 348, 118421	6	0
6	Thermodynamic modeling of calcium carbonate scale precipitation: aqueous Na ⁺ -Ca ²⁺ -Cl ⁻ -HCO ₃ ⁻ -CO ₃ ²⁻ -CO ₂ system. <i>Fluid Phase Equilibria</i> , 2021 , 113263	2.5	0
5	Batch-screening guided continuous flow synthesis of the metal-organic framework HKUST-1 in a millifluidic droplet reactor. <i>Microporous and Mesoporous Materials</i> , 2022 , 339, 112005	5.3	0
4	THERMODYNAMIC MODELING OF AQUEOUS AND MIXED SOLVENT ELECTROLYTE SYSTEMS 2019 , 493-504		
3	Industrial Applications of Plant-Wide Equation-Oriented Process Modeling 2010. <i>Advances in Chemical Engineering</i> , 2011 , 40, 119-152	0.6	

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1 Thermodynamic modeling of aqueous polyelectrolyte solutions with mixed-valent counterions. *Journal of Chemical Thermodynamics*, **2022**, 169, 106761 2.9