Frederico Wanderley Tavares

List of Publications by Year
in descending order

183	3,396	185998 28	189595 50
papers	citations	h-index	g-index

190	190	190	2796
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Why forces between proteins follow different Hofmeister series for pH above and below pI. Biophysical Chemistry, 2005, 117, 217-224.	1.5	194
2	Thermodynamics of fluid-phase equilibria for standard chemical engineering operations. AICHE Journal, 2004, 50, 739-761.	1.8	183
3	Influence of particle shape on the packing and on the segregation of spherocylinders via Monte Carlo simulations. Powder Technology, 2003, 134, 167-180.	2.1	165
4	Ion-Specific Effects in the Colloidâ^'Colloid or Proteinâ^'Protein Potential of Mean Force:Â Role of Saltâ^'Macroion van der Waals Interactions. Journal of Physical Chemistry B, 2004, 108, 9228-9235.	1.2	142
5	Thermodynamic modeling of confined fluids using an extension of the generalized van der Waals theory. Chemical Engineering Science, 2010, 65, 3088-3099.	1.9	135
6	Phase equilibrium of fluids confined in porous media from an extended Pengâ€“Robinson equation of state. Fluid Phase Equilibria, 2014, 362, 335-341.	1.4	122
7	Critical behavior of pure confined fluids from an extension of the van der Waals equation of state. Journal of Supercritical Fluids, 2010, 55, 455-461.	1.6	101
8	Phase behavior of soybean oil, castor oil and their fatty acid ethyl esters in carbon dioxide at high pressures. Journal of Supercritical Fluids, 2006, 37, 29-37.	1.6	98
9	Equation of state for the square-well chain fluid based on the dimer version of Wertheim's perturbation theory. Molecular Physics, 1995, 86, 1451-1471.	0.8	68
10	Hofmeister effects: Why protein charge, pH titration and protein precipitation depend on the choice of background salt solution. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2006, 282-283, 457-463.	2.3	58
11	Specific Ion Effects in Solutions of Globular Proteins:Â Comparison between Analytical Models and Simulation. Journal of Physical Chemistry B, 2005, 109, 24489-24494.	1.2	52
12	Machine learning model and optimization of a PSA unit for methane-nitrogen separation. Computers and Chemical Engineering, 2017, 104, 377-391.	2.0	51
13	A completely analytic equation of state for the square-well chain fluid of variable well width. Fluid Phase Equilibria, 1997, 140, 129-143.	1.4	50
14	Phase behavior of olive and soybean oils in compressed propane and n-butane. Brazilian Journal of Chemical Engineering, 2006, 23, 405-415.	0.7	48
15	Specific Ion Adsorption and Surface Forces in Colloid Science. Journal of Physical Chemistry B, 2008, 112, 1580-1585.	1.2	48
16	Effect of Salt Identity on the Phase Diagram for a Globular Protein in Aqueous Electrolyte Solution. Journal of Physical Chemistry B, 2006, 110, 24757-24760.	1.2	44
17	Analytic calculation of phase diagrams for solutions containing colloids or globular proteins. Colloid and Polymer Science, 2004, 282, 620-632.	1.0	41
18	Current status of Lattice Boltzmann Methods applied to aerodynamic, aeroacoustic, and thermal flows. Progress in Aerospace Sciences, 2020, 115, 100616.	6.3	38

#	Article	IF	Citations
19	Osmotic Second Virial Coefficients and Phase Diagrams for Aqueous Proteins from a Much-Improved Poissonâ^'Boltzmann Equationâ€. Journal of Physical Chemistry C, 2007, 111, 16055-16059.	1.5	36
20	Calculations of thermodynamic equilibrium in systems subject to gravitational fields. Chemical Engineering Science, 2000, 55, 3495-3504.	1.9	35
21	Vapor Pressure Data of Soybean Oil, Castor Oil, and Their Fatty Acid Ethyl Ester Derivatives. Journal of Chemical & Engineering Data, 2005, 50, 330-333.	1.0	34
22	Molecular Dynamic Simulation of Oxaliplatin Diffusion in Poly(lactic acid-co -glycolic acid). Part A: Parameterization and Validation of the Force-Field CVFF. Macromolecular Theory and Simulations, 2016, 25, 45-62.	0.6	34
23	Phase behavior of aqueous solutions containing dipolar proteins from second-order perturbation theory. Journal of Chemical Physics, 2004, 120, 9859-9869.	1.2	33
24	Methane/nitrogen separation through pressure swing adsorption process from nitrogen-rich streams. Chemical Engineering and Processing: Process Intensification, 2016, 103, 70-79.	1.8	33
25	Liquid film flow and area generation in structured packed columns. Powder Technology, 1999, 104, 84-94.	2.1	31
26	High-Pressure Experimental Data of CO₂ + Mitotane and CO₂ + Ethanol + Mitotane Mixtures. Journal of Chemical & Engineering Data, 2011, 56, 4333-4341.	1.0	31
27	Phase behavior of castor oil in compressed propane and n-butane. Journal of Supercritical Fluids, 2005, 34, 215-221.	1.6	30
28	Investigation of adsorption-enhanced reaction process of mercury removal from simulated natural gas by mathematical modeling. Fuel, 2014, 129, 129-137.	3.4	30
29	Group contribution equation of state based on the lattice fluid theory: Alkaneâ€“alkanol systems. Fluid Phase Equilibria, 1998, 142, 33-54.	1.4	29
30	MOLECULAR THERMODYNAMICS OF MICELLIZATION: MICELLE SIZE DISTRIBUTIONS AND GEOMETRY TRANSITIONS. Brazilian Journal of Chemical Engineering, 2016, 33, 515-523.	0.7	29
31	Sixty Years of the van der Waals and Platteeuw Model for Clathrate Hydratesâ€”A Critical Review from Its Statistical Thermodynamic Basis to Its Extensions and Applications. Chemical Reviews, 2020, 120, 13349-13381.	23.0	29
32	The role of saltâ€“macroion van der Waals interactions in the colloidâ€“colloid potential of mean force. Current Opinion in Colloid and Interface Science, 2004, 9, 81-86.	3.4	27
33	Phase equilibria of polypropylene samples with hydrocarbon solvents at high pressures. Journal of Applied Polymer Science, 2001, 81, 3044-3055.	1.3	26
34	Finite volume solution of the modified Poissonâ€“Boltzmann equation for two colloidal particles. Physical Chemistry Chemical Physics, 2007, 9, 3174-3180.	1.3	26
35	New Cascaded Thermal Lattice Boltzmann Method for simulations of advection-diffusion and convective heat transfer. International Journal of Thermal Sciences, 2017, 118, 259-277.	2.6	26
36	Co-Ion and Ion Competition Effects:â€‰ Ion Distributions Close to a Hydrophobic Solid Surface in Mixed Electrolyte Solutions. Langmuir, 2008, 24, 3944-3948.	1.6	25

#	Article	IF	Citations
37	Lattice Boltzmann Methods for Industrial Applications. Industrial & Engineering Chemistry Research, 2019, 58, 16205-16234.	1.8	25
38	Amorphous paracrystalline structures from native crystalline cellulose: A molecular dynamics protocol. Fluid Phase Equilibria, 2019, 491, 56-76.	1.4	25
39	The influence of ion binding and ion specific potentials on the double layer pressure between charged bilayers at low salt concentrations. Journal of Chemical Physics, 2008, 128, 135104.	1.2	23
40	Molecular dynamics simulation data of self-diffusion coefficient for Lennardâ€“Jones chain fluids. Fluid Phase Equilibria, 2004, 221, 25-33.	1.4	22
41	Thermodynamic equilibrium in systems with multiple adsorbed and bulk phases. Chemical Engineering Science, 2005, 60, 1773-1782.	1.9	22
42	Extending an equation of state to confined fluids with basis on molecular simulations. Chemical Engineering Science, 2016, 153, 212-220.	1.9	22
43	Cure kinetic parameter estimation of thermosetting resins with isothermal data by using particle swarm optimization. European Polymer Journal, 2008, 44, 2678-2686.	2.6	21
44	Thermodynamic Properties of 1:1 Salt Aqueous Solutions with the Electrolattice Equation of State. Oil and Gas Science and Technology, 2013, 68, 255-270.	1.4	21
45	Are all-atom any better than united-atom force fields for the description of liquid properties of alkanes?. Journal of Molecular Modeling, 2020, 26, 296.	0.8	21
46	Self- and mutual diffusion coefficient equation for pure fluids, liquid mixtures and polymeric solutions. Chemical Engineering Science, 2005, 60, 4581-4592.	1.9	19
47	Stability studies of high-stable water-in-oil model emulsions. Journal of Dispersion Science and Technology, 2017, 38, 82-88.	1.3	19
48	Cubic equations of state extended to confined fluids: New mixing rules and extension to spherical pores. Chemical Engineering Science, 2018, 184, 52-61.	1.9	19
49	Phase behavior of isotactic polypropylene/C4-solvents at high pressure. Experimental data and SAFT modeling. Journal of Supercritical Fluids, 2001, 21, 93-103.	1.6	18
50	Specific ion effects: Interaction between nanoparticles in electrolyte solutions. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2008, 319, 98-102.	2.3	18
51	Double layer interaction between charged parallel plates using a modified Poissonâ€“Boltzmann equation to include size effects and ion specificity. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2012, 412, 29-35.	2.3	18
52	Development of an AMBER-compatible transferable force field for poly(ethylene glycol) ethers (glymes). Journal of Molecular Modeling, 2017, 23, 194.	0.8	17
53	Effect of the ion-protein dispersion interactions on the protein-surface and protein-protein interactions. Journal of the Brazilian Chemical Society, 2007, 18, 223-230.	0.6	16
54	Emulsion phase inversion of model and crude oil systems detected by near-infrared spectroscopy and principal component analysis. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2018, 538, 565-573.	2.3	16

#	Article	IF	Citations
55	Natural convection heat transfer modeling by the cascaded thermal lattice Boltzmann method. International Journal of Thermal Sciences, 2018, 134, 552-564.	2.6	16
56	RESEARCH NOTE Vapour-liquid equilibria of exponential-six fluids. Molecular Physics, 1996, 87, 1471-1476.	0.8	16
57	Monte Carlo simulation of particle segregation. Powder Technology, 1998, 97, 200-207.	2.1	15
58	Analytic calculation of phase diagrams for charged dipolar colloids with orientation-averaged pair potentials. Physical Chemistry Chemical Physics, 2003, 5, 4851.	1.3	15
59	High-pressure phase diagram of the drug mitotane in compressed and/or supercritical CO2. Journal of Chemical Thermodynamics, 2010, 42, 286-290.	1.0	15
60	Cubic Plus Association Equation of State for Flow Assurance Projects. Industrial & Engineering Chemistry Research, 2015, 54, 6812-6824.	1.8	15
61	Monte Carlo Simulations of the Adsorption of Chainlike Molecules on Two-Dimensional Heterogeneous Surfaces. Langmuir, 2003, 19, 1429-1438.	1.6	14
62	Phase transition of waterâ€“inâ€“oil emulsions over influence of an external electric field. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2008, 326, 10-17.	2.3	14
63	Anion-Specific Partitioning in Two-Phase Finite Volume Systems: Possible Implications for Mechanisms of Ion Pumps. Journal of Physical Chemistry B, 2009, 113, 8124-8127.	1.2	14
64	Evaluation of Microwave and Conventional Heating for Electrostatic Treatment of a Water-in-Oil Model Emulsion in a Pilot Plant. Energy & Fuels, 2017, 31, 6587-6597.	2.5	14
65	Self-diffusion coefficients of methane/n-hexane mixtures at high pressures: An evaluation of the finite-size effect and a comparison of force fields. Journal of Supercritical Fluids, 2020, 155, 104639.	1.6	14
66	Transitional Phase Inversion of Emulsions Monitored by in Situ Near-Infrared Spectroscopy. Langmuir, 2013, 29, 5995-6003.	1.6	13
67	A new simple and efficient flash algorithm for T-v specifications. Fluid Phase Equilibria, 2018, 464, 32-39.	1.4	13
68	Square-well chain mixture: analytic equation of state and Monte Carlo simulation data. Fluid Phase Equilibria, 2001, 179, 245-267.	1.4	12
69	Role of attractive forces in self-diffusion and mutual diffusion in dense simple fluids and real substances. Fluid Phase Equilibria, 2002, 194-197, 1131-1140.	1.4	12
70	Concentration and Solvent Effects on Structural, Dynamical, and Rheological Properties of Asphaltene Suspensions. Energy & Fuels, 2020, 34, 1071-1081.	2.5	12
71	Asphaltenes at the water-oil interface using DPD/COSMO-SAC. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2021, 625, 126828.	2.3	12
72	Dense fluid self-diffusion coefficient calculations using perturbation theory and molecular dynamics. Brazilian Journal of Chemical Engineering, 1999, 16, 319-329.	0.7	12

#	Article	IF	Citations
73	A Monte Carlo simulation of the packing and segregation of spheres in cylinders. Brazilian Journal of Chemical Engineering, 1999, 16, 395-405.	0.7	12
74	Ion specific forces between charged self-assembled monolayers explained by modified DLVO theory. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2009, 346, 11-15.	2.3	11
75	NON-EQUILIBRIUM MOLECULAR DYNAMICS USED TO OBTAIN SORET COEFFICIENTS OF BINARY HYDROCARBON MIXTURES. Brazilian Journal of Chemical Engineering, 2015, 32, 683-698.	0.7	11
76	Effects of electrostatic correlations on ion dynamics in alternating current voltages. Electrochimica Acta, 2015, 152, 84-92.	2.6	11
77	Simultaneous multiphase flash and stability analysis calculations including hydrates. Fluid Phase Equilibria, 2016, 413, 196-208.	1.4	11
78	Accurate thermodynamic description of vaporâ€“liquid and solidâ€“liquid equilibria of THF, water and gas hydrates with a unique set of parameters. Journal of Chemical Thermodynamics, 2018, 117, 60-67.	1.0	11
79	A molecular dynamics study of the solvation of carbon dioxide and other compounds in the ionic liquids [emim][B(CN)4] and [emim][NTf2]. Fluid Phase Equilibria, 2019, 491, 1-11.	1.4	11
80	Vapour-liquid equilibria of exponential-six fluids. Molecular Physics, 1996, 87, 1471-1476.	0.8	10
81	An Equation of State for Polymers and Normal Fluids Using the Square-Well Potential of Variable Well Width. Industrial & Engineering Chemistry Research, 2001, 40, 1748-1754.	1.8	10
82	Parameter estimation of kinetic cure using DSC non-isothermal data. Journal of Thermal Analysis and Calorimetry, 2011, 103, 495-499.	2.0	10
83	Studies on transitional emulsion phase inversion using the steady state protocol. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2015, 484, 424-433.	2.3	10
84	The impact of the adsorbent energy heterogeneities by multidimensional-multicomponent PC-SAFT-DFT. Fluid Phase Equilibria, 2022, 562, 113546.	1.4	10
85	An analytic equation-of-state for mixture of square-well chain fluids of variable well width. Fluid Phase Equilibria, 2001, 179, 231-243.	1.4	9
86	Centrifugation equilibrium of natural gas. Chemical Engineering Science, 2005, 60, 2927-2935.	1.9	9
87	Steric effects on ion dynamics near charged electrodes. Fluid Phase Equilibria, 2014, 362, 177-186.	1.4	9
88	Membrane Potential and Ion Partitioning in an Erythrocyte Using the Poissonâ€“Boltzmann Equation. Journal of Physical Chemistry B, 2015, 119, 6379-6388.	1.2	9
89	Crude Oil Electrical Conductivity Measurements at High Temperatures: Introduction of Apparatus and Methodology. Energy & Fuels, 2017, 31, 3669-3674.	2.5	9
90	A modified Poisson-Boltzmann equation applied to protein adsorption. Journal of Chromatography A, 2018, 1531, 74-82.	1.8	9

#	Article	IF	Citations
91	Forces between air-bubbles in electrolyte solution. Chemical Physics Letters, 2008, 458, 299-302.	1.2	8
92	Attractive double-layer forces between neutral hydrophobic and neutral hydrophilic surfaces. Physical Review E, 2011, 84, 061903.	0.8	8
93	The electrostatic behavior of the bacterial cell wall using a smoothing function to describe the charge-regulated volume charge density profile. Colloids and Surfaces B: Biointerfaces, 2015, 134, 447-452.	2.5	8
94	Non-isothermal population balance model of the formation and dissociation of gas hydrates. Chemical Engineering Science, 2017, 163, 234-254.	1.9	8
95	Effect of electrostatic correlations on micelle formation. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2017, 533, 169-178.	2.3	8
96	High pressure phase equilibria of carbon dioxideÂ+Ân-alkanes mixtures: Experimental data and modeling. Fluid Phase Equilibria, 2018, 463, 114-120.	1.4	8
97	Representative elementary volume in limestone sample. Journal of Instrumentation, 2018, 13, C10003-C10003.	0.5	8
98	Pore size distributions from extended Peng-Robinson equations of state for fluids confined in cylindrical and slit pores. Fluid Phase Equilibria, 2019, 493, 67-77.	1.4	8
99	Phase Equilibria Data and Thermodynamic Analysis for Liquidâ€“Hydrateâ€“Vapor (LHV) with High Ethanol Concentrations. Journal of Chemical & Engineering Data, 2020, 65, 349-359.	1.0	8
100	Quenched solid density functional theory coupled with PC-SAFT for the adsorption modeling on nanopores. Fluid Phase Equilibria, 2020, 521, 112700.	1.4	8
101	Monte Carlo simulation of adsorption using 2-D models of heterogeneous solids. AICHE Journal, 2003, 49, 753-763.	1.8	7
102	Shear viscosity calculated by perturbation theory and molecular dynamics for dense fluids. International Journal of Quantum Chemistry, 2003, 95, 79-87.	1.0	7
103	Thermodynamic equilibrium of adsorbed phases. Fluid Phase Equilibria, 2005, 233, 66-72.	1.4	7
104	Ion-Specific Forces between a Colloidal Nanoprobe and a Charged Surface. Langmuir, 2007, 23, 7456-7458.	1.6	7
105	Modeling MEA with the CPA equation of state: A parameter estimation study adding local search to PSO algorithm. Fluid Phase Equilibria, 2015, 400, 76-86.	1.4	7
106	Molecular Modeling in Chemical Engineering. , 2017, , .		7
107	A First Approach towards Adsorption-Oriented Physics-Informed Neural Networks: Monoclonal Antibody Adsorption Performance on an Ion-Exchange Column as a Case Study. ChemEngineering, 2022, 6, 21.	1.0	7
108	Equations of state for chainlike polar fluids: a comparison of reference terms. Fluid Phase Equilibria, 1994, 99, 87-103.	1.4	6

#	Article	IF	Citations
109	Phase equilibrium calculations for confined fluids, including surface tension prediction models. Brazilian Journal of Chemical Engineering, 2005, 22, 93-104.	0.7	6
110	Vaporâ€“liquid equilibrium calculations for refrigerant mixtures with the Mattediâ€“Tavaresâ€“Castier EOS. Fluid Phase Equilibria, 2010, 296, 133-139.	1.4	6
111	Influence of Commercial Anti-agglomerants and Ammonium Quaternary Compounds on the Stability of Waxy Crude Oil Emulsion. Energy & Fuels, 2015, 29, 2211-2218.	2.5	6
112	A modified multi-site occupancy model: evaluation of azeotropelike behavior in adsorption. Adsorption, 2015, 21, 3-16.	1.4	6
113	Alternative EoS-based model for predicting water content, metastable phases and hydrate formation in natural gas systems. Journal of Natural Gas Science and Engineering, 2016, 36, 550-562.	2.1	6
114	Phase diagrams for hydrates beyond incipient condition â€” Complex behavior in methane/propane and carbon dioxide/iso-butane hydrates. Fluid Phase Equilibria, 2016, 426, 75-82.	1.4	6
115	Equation of state based on the hole-lattice theory and surface-charge density (COSMO): Part A â€“ Pure compounds. Fluid Phase Equilibria, 2016, 409, 472-481.	1.4	6
116	Phenomenological modeling for elemental mercury capture on hydroxyapatite-based adsorbents: An experimental validation. Fuel, 2018, 225, 509-518.	3.4	6
117	A computational tool for parameter estimation in EoS: New methodologies and natural gas phase equilibria calculations. Chemical Engineering Science, 2020, 215, 115437.	1.9	6
118	Phase behavior of systems with high CO2 content: Experiments and thermodynamic modeling. Fluid Phase Equilibria, 2020, 515, 112574.	1.4	6
119	Synthesis of polyglobalide by enzymatic ring opening polymerization using pressurized fluids. Journal of Supercritical Fluids, 2022, 186, 105588.	1.6	6
120	A phase stability analysis of the combinatorial term of the UNIQUAC model. Chemical Engineering Science, 1999, 54, 893-896.	1.9	5
121	Centrifugation equilibrium for spheres and spherocylinders. Journal of Colloid and Interface Science, 2005, 281, 360-367.	5.0	5
122	Modeling Water Saturation Points in Natural Gas Streams Containing CO₂ and H₂Sâ€”Comparisons with Different Equations of State. Industrial & Engineering Chemistry Research, 2015, 54, 743-757.	1.8	5
123	Molecular dynamics simulation and experimental validation by X-ray data of hydroxyapatite crystalline structures. Fluid Phase Equilibria, 2018, 470, 60-67.	1.4	5
124	Reconstruction of the pore size distribution of porous materials: The influence of uncertainties in the gaseous adsorption experimental data. Fluid Phase Equilibria, 2019, 494, 93-102.	1.4	5
125	Wax appearance and prevention in two-phase flow using the multi-solid and drift-flux model. Journal of Petroleum Science and Engineering, 2019, 177, 374-383.	2.1	5
126	Renormalization group theory applied to the CPA equation of state: Impacts on phase equilibrium and derivative properties. Fluid Phase Equilibria, 2020, 506, 112365.	1.4	5

#	Article	IF	Citations
127	Development of Coalescence and Capture Kernels for the Electrocoalescence Process Based on Batch Experiments. Industrial & Engineering Chemistry Research, 2020, 59, 1277-1297.	1.8	5
128	Modified clustering algorithm for molecular simulation. Molecular Simulation, 2020, 46, 1453-1466.	0.9	5
129	Exploring the multiple solutions of the classical density functional theory using metadynamics based method. Adsorption, 2021, 27, 1023-1034.	1.4	5
130	Molecular dynamics of dissolution of a 36-chain cellulose Iβ microfibril at different temperatures above the critical pressure of water. Journal of Molecular Liquids, 2021, 336, 116271.	2.3	5
131	PCP-SAFT Density Functional Theory as a much-improved approach to obtain confined fluid isotherm data applied to sub and supercritical conditions. Chemical Engineering Science, 2022, 247, 116905.	1.9	5
132	GROUP CONTRIBUTION LATTICE FLUID EQUATION OF STATE: APPLICATION TO POLYMER+SOLVENT SYSTEMS. Brazilian Journal of Chemical Engineering, 1998, 15, 313-319.	0.7	5
133	Phase equilibria of binary mixtures by molecular simulation and cubic equations of state. Brazilian Journal of Chemical Engineering, 2001, 18, 149-161.	0.7	5
134	Are all-atom any better than united-atom force fields for the description of liquid properties of alkanes? 2. A systematic study considering different chain lengths. Journal of Molecular Liquids, 2022, 354, 118829.	2.3	5
135	Adsorption equilibrium of light hydrocarbon mixtures by monte carlo simulation. Brazilian Journal of Chemical Engineering, 2007, 24, 597-610.	0.7	4
136	Vaporâ˜'Liquid Equilibrium Calculations of Aqueous and Nonaqueous Binary Systems Using the Mattediâ˜'Tavaresâ˜'Castier Equation of State. Industrial & Engineering Chemistry Research, 2011, 50, 102-110.	1.8	4
137	A lowâ€disturbance nonequilibrium molecular dynamics algorithm applied to the determination of thermal conductivities. AICHE Journal, 2015, 61, 2881-2890.	1.8	4
138	Investigation of the PIT emulsification mechanism by NIR and conductometry. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2016, 506, 566-575.	2.3	4
139	CHEMICAL POTENTIALS OF HARD-CORE MOLECULES BY A STEPWISE INSERTION METHOD. Brazilian Journal of Chemical Engineering, 2018, 35, 277-288.	0.7	4
140	Paraffin solubility curves of diesel fuels from thermodynamic model adjusted through experimental DSC thermograms. Fuel, 2018, 230, 266-273.	3.4	4
141	Laser-induced alteration of microstructural and microscopic transport properties in porous materials: Experiment, modeling and analysis. Materials and Design, 2018, 155, 307-316.	3.3	4
142	Adsorption of Gases on Zeolitic Imidazolate Frameworks: Modeling with Equations of State for Confined Fluids and Pore Size Distribution Estimation. Industrial & Engineering Chemistry Research, 2019, 58, 19702-19708.	1.8	4
143	Experimental high-pressure phase equilibria of carbon dioxide/n-alkanes mixtures and model-parameters for solid-phase obtained from DSC thermograms. Fluid Phase Equilibria, 2020, 526, 112802.	1.4	4
144	Thermophysical Properties of Amorphousâ€Paracrystalline Celluloses by Molecular Dynamics. Macromolecular Theory and Simulations, 2020, 29, 2000007.	0.6	4

#	Article	IF	Citations
145	Helmholtz Scaling: An Alternative Approach to Calculate Viscosity with the PCP-SAFT Equation of State. Industrial & Engineering Chemistry Research, 2021, 60, 9231-9245.	1.8	4
146	The binding interaction of protein on a charged surface using Poissonâ€“Boltzmann equation: lysozyme adsorption onto SBA-15. Adsorption, 2021, 27, 1137-1148.	1.4	4
147	Phase Equilibrium Calculations for Semicontinuous Mixtures Subject to Gravitational Fields. Industrial & Engineering Chemistry Research, 2000, 39, 4415-4421.	1.8	3
148	High pressure phase equilibrium calculations for hydrocarbon systems using an equation of state based on the lattice fluid theory. Fluid Phase Equilibria, 2002, 194-197, 599-607.	1.4	3
149	Improving the SAFT-EOS by using an effective WCA segment diameter. Fluid Phase Equilibria, 2002, 194-197, 531-539.	1.4	3
150	Evaluation of mixing and combining rules for asymmetric Lennardâ€“Jones chain mixtures: Effect of segment diameter, energy interaction, and chain length. Fluid Phase Equilibria, 2007, 259, 123-134.	1.4	3
151	Ion-specific thermodynamic properties of colloids and proteins. Fluid Phase Equilibria, 2010, 296, 99-105.	1.4	3
152	Ion-specific thermodynamical properties of aqueous proteins. Anais Da Academia Brasileira De Ciencias, 2010, 82, 109-126.	0.3	3
153	Paraffin solubility and calorimetric data calculation using Peng-Robinson EoS and modified UNIQUAC models. Journal of Petroleum Science and Engineering, 2017, 156, 945-957.	2.1	3
154	Heat of dissociation from Statistical Thermodynamics: Using calorimetric data to estimate gas hydrate parameters. Journal of Chemical Thermodynamics, 2018, 117, 164-179.	1.0	3
155	A new high-pressure cell for equilibrium measurements of systems with fluid and solid phases. Journal of Supercritical Fluids, 2022, 179, 105420.	1.6	3
156	Calculation of mixture critical diagrams using an equation of state based on the lattice fluid theory. Brazilian Journal of Chemical Engineering, 2000, 17, 771-784.	0.7	3
157	Calculation of sedimentation equilibrium using a modified flash algorithm. Chemical Engineering Science, 2001, 56, 3771-3779.	1.9	2
158	Mutual diffusion coefficient models for polymer-solvent systems based on the Chapman-Enskog theory. Brazilian Journal of Chemical Engineering, 2004, 21, 611-619.	0.7	2
159	Inner segment radial distribution functions at contact point for chain-like molecules. Journal of Molecular Liquids, 2009, 147, 198-210.	2.3	2
160	Modelling of Hg⁰ Removal from Gaseous Streams and its Fixation in Hydroxyapatite-Based Adsorbents Modified with Copper Sulphide. Adsorption Science and Technology, 2015, 33, 175-190.	1.5	2
161	Equation of state based on the hole-lattice theory and surface-charge density (COSMO): Part B â€“ Vaporâ€“liquid equilibrium for mixtures. Fluid Phase Equilibria, 2016, 419, 1-10.	1.4	2
162			

#	Article	IF	Citations
163	Phase Equilibrium Thermodynamics. , 2017, , 35-80.		2
164	Laser-induced wettability alteration in limestone rocks. Materials Today Communications, 2018, 17, 332-340.	0.9	2
165	Cascaded Lattice Boltzmann Method application in forced and natural convection. Journal of Physics: Conference Series, 2018, 1101, 012040.	0.3	2
166	Wettability of rock, oil and brine system based on density functional theory. Fluid Phase Equilibria, 2019, 479, 99-105.	1.4	2
167	Anomalous diffusion and sorption-desorption process in complex fluid systems. Communications in Nonlinear Science and Numerical Simulation, 2020, 90, 105411.	1.7	2
168	Molecular Thermodynamics for Aggregation of Surfactants with Alkylbenzene or Branched Alkane Tails: An Experimental-Modeling Approach. Fluid Phase Equilibria, 2021, 532, 112918.	1.4	2
169	MONTE CARLO SIMULATIONS OF THE ADSORPTION OF DIMERS ON STRUCTURED HETEROGENEOUS SURFACES. Brazilian Journal of Chemical Engineering, 2001, 18, 385-397.	0.7	2
170	Microscope analysis and evaluation of the destabilization process of water-in-oil emulsions under application of electric field. IEEE Transactions on Dielectrics and Electrical Insulation, 2020, 27, 873-881.	1.8	2
171	Modifying the Poissonâ€“Boltzmann Approach to Model Specific Ion Effects. , 2009, , 293-309.		1
172	A self-consistent perturbative density functional theory for hard-core fluids: phase diagrams, structural and interfacial properties. Fluid Phase Equilibria, 2021, 542-543, 113095.	1.4	1
173	Ion Specific Interactions Between Pairs of Nanometer Sized Particles in Aqueous Solutions. , 2006, , 74-77.		1
174	STEADY STATE AND PSEUDO-TRANSIENT ELECTRIC POTENTIAL USING THE POISSONBOLTZMANN EQUATION. Brazilian Journal of Chemical Engineering, 2015, 32, 293-302.	0.7	1
175	A comparison of simulated annealing algorithms in the scheduling of multiproduct serial batch plants. Brazilian Journal of Chemical Engineering, 2000, 17, 199-209.	0.7	1
176	Rheological Behavior of an Epoxy Resin with Hollow Glass Microspheres. AIP Conference Proceedings, 2008, , .	0.3	0
177	Ion-specific potential of mean force between two aqueous proteins. Computer Aided Chemical Engineering, 2008, , 865-870.	0.3	0
178	Phase Equilibrium Under the Influence of the Gravitational Field. , 2017, , 81-101.		0
179	General Comments and Perspectives. , 2017, , 239-245.		0
180	Electro-rheological investigation on W/O emulsions morphology under electric fields. Journal of Dispersion Science and Technology, 2020, 41, 1465-1470.	1.3	0

#	Article	IF	Citations
181	Inferring kinetic dissolution of NaCl in aqueous glycol solution using a lowâ€cost apparatus and population balance model. Canadian Journal of Chemical Engineering, 2020, 98, 2435-2450.	0.9	0
182	Physicalâ€“Chemical Properties of Compressible Clathrates: A Natural Pressure Shift by Extending the van der Waals and Platteeuw Model. Journal of Physical Chemistry C, 2022, 126, 2839-2856.	1.5	0
183	Revisiting the birth of NaCl crystals using molecular dynamics simulation. Journal of Molecular Graphics and Modelling, 2022, 115, 108202.	1.3	0