Vincent Gerbaud

List of Publications by Year
in descending order

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130 papers	2,909 citations	172207 29 h-index	205818 48 g-index
133 all docs	133 docs citations	133 times ranked	1577 citing authors

#	Article	IF	Citations
1	Selection of green solvents for organic photovoltaics by reverse engineering. Molecular Systems Design and Engineering, 2022, 7, 182-195.	1.7	1
2	Bibliometric survey and network analysis of biomimetics and nature inspiration in engineering science. Bioinspiration and Biomimetics, 2022, 17, 031001.	1.5	4
3	Bio-Refinery of Oilseeds: Oil Extraction, Secondary Metabolites Separation towards Protein Meal Valorisationâ€”A Review. Processes, 2022, 10, 841.	1.3	17
4	A nonequilibrium thermodynamics perspective on nature-inspired chemical engineering processes. Chemical Engineering Research and Design, 2020, 154, 316-330.	2.7	10
5	Accurate hydrogenated vegetable oil viscosity predictions for monolith reactor simulations. Chemical Engineering Science, 2020, 214, 115388.	1.9	6
6	Flash point prediction with UNIFAC type models of ethylic biodiesel and binary/ternary mixtures of FAEEs. Fuel, 2020, 281, 118717.	3.4	18
7	Impact of taxes and investment incentive on the development of renewable energy self-consumption: French householdsâ€™ case study. Journal of Cleaner Production, 2020, 265, 121791.	4.6	9
8	Controlling Solvation and Mass Transport Properties of Biobased Solvents through CO₂ Expansion: A Physicochemical and Molecular Modeling Study. Industrial & Engineering Chemistry Research, 2019, 58, 18942-18964.	1.8	7
9	Fundamentals of Equilibrium Thermodynamics. , 2019, , 1-85.		4
10	CAMD for entrainer screening of extractive distillation process based on new thermodynamic criteria. Chemical Engineering Research and Design, 2019, 147, 721-733.	2.7	19
11	Interfacially driven transport theory: a way to unify Marangoni and osmotic flows. Physical Chemistry Chemical Physics, 2019, 21, 10114-10124.	1.3	4
12	Modelling and experimental validation of dimethyl carbonate solvent recovery from an aroma mixture by batch distillation. Chemical Engineering Research and Design, 2019, 147, 1-17.	2.7	3
13	A flexible metamodel architecture for optimal design of Hybrid Renewable Energy Systems (HRES) â€“ Case study of a stand-alone HRES for a factory in tropical island. Journal of Cleaner Production, 2019, 223, 214-225.	4.6	26
14	Review of extractive distillation. Process design, operation, optimization and control. Chemical Engineering Research and Design, 2019, 141, 229-271.	2.7	162
15	Design and control of pressureâ€swing distillation for separating ternary systems with three binary minimum azeotropes. AICHE Journal, 2019, 65, 1281-1293.	1.8	167
16	Advances in Extractive Distillation. , 2019, , .		6
17	CO₂-Expanded Alkyl Acetates: Physicochemical and Molecular Modeling Study and Applications in Chemical Processes. ACS Sustainable Chemistry and Engineering, 2018, 6, 7627-7637.	3.2	8
18	Classification for ternary flash point mixtures diagrams regarding miscible flammable compounds. Fluid Phase Equilibria, 2018, 466, 110-123.	1.4	7

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19	Cyclic operation as optimal control reflux policy of binary mixture batch distillation. Computers and Chemical Engineering, 2018, 108, 98-111.	2.0	7
20	Optimization of pre-concentration, entrainer recycle and pressure selection for the extractive distillation of acetonitrile-water with ethylene glycol. Chemical Engineering Science, 2018, 177, 354-368.	1.9	83
21	Energy-Saving Reduced-Pressure Extractive Distillation with Heat Integration for Separating the Biazeotropic Ternary Mixture Tetrahydrofuranâ€“Methanolâ€“Water. Industrial & Engineering Chemistry Research, 2018, 57, 13498-13510.	1.8	52
22	Computer-aided product design of alternative solvents based on phase equilibrium synergism in mixtures. Comptes Rendus Chimie, 2018, 21, 606-621.	0.2	9
23	A new HPF specimen carrier adapter for the use of highâ€pressure freezing with cryoscanning electron microscope: two applications: stearic acid organization in a hydroxypropyl methylcellulose matrix and mice myocardium. Journal of Microscopy, 2018, 271, 255-265.	0.8	5
24	Computer aided framework for designing bio-based commodity molecules with enhanced properties. Chemical Engineering Science, 2017, 159, 177-193.	1.9	14
25	CO2-Expanded Alkyl Lactates: A Physicochemical and Molecular Modeling Study. Journal of Solution Chemistry, 2017, 46, 259-280.	0.6	16
26	Holistic framework for land settlement development project sustainability assessment: Comparison of El Hierro Island hydro wind project and Sivens dam project. Computers and Chemical Engineering, 2017, 100, 153-176.	2.0	9
27	Effect of carboxymethylcellulose on potassium bitartrate crystallization on model solution and white wine. Journal of Crystal Growth, 2017, 472, 54-63.	0.7	9
28	On the relation between azeotropic behavior and minimum / maximum flash point occurrences in binary mixtures of flammable compounds. Fluid Phase Equilibria, 2017, 452, 113-134.	1.4	10
29	A novel method for detecting and computing univolatility curves in ternary mixtures. Chemical Engineering Science, 2017, 173, 21-36.	1.9	10
30	An Improved Shortcut Design Method of Divided Wall Columns Exemplified by a Liquefied Petroleum Gas Process. Industrial & Engineering Chemistry Research, 2017, 56, 9710-9720.	1.8	11
31	Predicting the Surface Tension of Liquids: Comparison of Four Modeling Approaches and Application to Cosmetic Oils. Journal of Chemical Information and Modeling, 2017, 57, 2986-2995.	2.5	22
32	Batch distillation of binary mixtures: preliminary analysis of optimal control. IFAC-PapersOnLine, 2017, 50, 4899-4904.	0.5	3
33	Molecular Dynamics Simulations of Gas-Expanded Liquids. Computer Aided Chemical Engineering, 2017, , 175-180.	0.3	2
34	Univolatility curves in ternary mixtures: geometry and numerical computation. Computer Aided Chemical Engineering, 2017, 40, 229-234.	0.3	0
35	A Meta-ontology to Design Sustainable Project in a Competitive Stakeholderâ€™s Context. Computer Aided Chemical Engineering, 2017, , 1903-1908.	0.3	0
36	Establishment of Collaborative Networks â€“ A Model-Driven Engineering Approach Based on Thermodynamics. IFIP Advances in Information and Communication Technology, 2017, , 641-648.	0.5	0

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37	CONCEPTUAL DESIGN OF NON-IDEAL MIXTURE SEPARATION WITH LIGHT ENTRAINERS. Brazilian Journal of Chemical Engineering, 2016, 33, 1041-1053.	0.7	9
38	Stearic acid crystals stabilization in aqueous polymeric dispersions. Chemical Engineering Research and Design, 2016, 110, 220-232.	2.7	4
39	Polymer-plasticizer compatibility during coating formulation: A multi-scale investigation. Progress in Organic Coatings, 2016, 101, 195-206.	1.9	53
40	Reducing process cost and CO2 emissions for extractive distillation by double-effect heat integration and mechanical heat pump. Applied Energy, 2016, 166, 128-140.	5.1	113
41	Low pressure design for reducing energy cost of extractive distillation for separating diisopropyl ether and isopropyl alcohol. Chemical Engineering Research and Design, 2016, 109, 540-552.	2.7	50
42	A â€œtop-downâ€•in silico approach for designing ad hoc bio-based solvents: application to glycerol-derived solvents of nitrocellulose. Green Chemistry, 2016, 18, 3239-3249.	4.6	28
43	Structure of aqueous colloidal formulations used in coating and agglomeration processes: Mesoscale model and experiments. Powder Technology, 2016, 291, 244-261.	2.1	6
44	Thermodynamic modeling of the condensable fraction of a gaseous effluent from lignocellulosic biomass torrefaction. Fluid Phase Equilibria, 2016, 409, 242-255.	1.4	13
45	Influence of wine polysaccharides and polyphenols on the crystallization of potassium hydrogen tartrate. Oeno One, 2016, 31, 65.	0.7	10
46	Study of wine tartaric acid salt stabilization by addition of carboxymethylcellulose (CMC): comparison with the Â« protective colloids Â» effect. Oeno One, 2016, 44, 231.	0.7	10
47	Systematic design of an extractive distillation for maximumâ€boiling azeotropes with heavy entrainers. AIChE Journal, 2015, 61, 3898-3910.	1.8	106
48	Glycerol acetals and ketals as bio-based solvents: positioning in Hansen and COSMO-RS spaces, volatility and stability towards hydrolysis and autoxidation. Green Chemistry, 2015, 17, 1779-1792.	4.6	59
49	Extractive distillation: recent advances in operation strategies. Reviews in Chemical Engineering, 2015, 31, .	2.3	26
50	Novel Procedure for Assessment of Feasible Design Parameters of Dividing-Wall Columns: Application to Non-azeotropic Mixtures. Industrial & Engineering Chemistry Research, 2015, 54, 5307-5318.	1.8	17
51	Investigation of Separation Efficiency Indicator for the Optimization of the Acetoneâ€“Methanol Extractive Distillation with Water. Industrial & Engineering Chemistry Research, 2015, 54, 10863-10875.	1.8	31
52	On the Riemannian structure of the residue curves maps. Chemical Engineering Research and Design, 2015, 99, 87-96.	2.7	2
53	Improved Design and Efficiency of the Extractive Distillation Process for Acetoneâ€“Methanol with Water. Industrial & Engineering Chemistry Research, 2015, 54, 491-501.	1.8	59
54	Prediction of solidâ€“binder affinity in dry and aqueous systems: Work of adhesion approach vs. ideal tensile strength approach. Powder Technology, 2015, 271, 61-75.	2.1	12

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55	Ternary Blends of Vegetable Oils: Thermal Profile Predictions for Product Design. Computer Aided Chemical Engineering, 2014, 33, 1465-1470.	0.3	2
56	Beyond biofuels: economic opportunities, recent advances and challenges in property modeling for vegetable oils. Green Processing and Synthesis, 2014, 3, 401-410.	1.3	8
57	From chemical platform molecules to new biosolvents: Design engineering as a substitution methodology. Biofuels, Bioproducts and Biorefining, 2014, 8, 438-451.	1.9	21
58	Classification of the Aroma Quality of Pyrazine Derivatives using Random Forest Tree Technique. , 2014, , 499-502.		0
59	Solid Fat Content of vegetable oils and simulation of interesterification reaction: Predictions from thermodynamic approach. Journal of Food Engineering, 2014, 126, 198-205.	2.7	31
60	Chemical enterprise model and decision-making framework for sustainable chemical product design. Computers in Industry, 2014, 65, 505-520.	5.7	34
61	General Model for Studying the Feasibility of Heterogeneous Extractive Batch Distillation. Industrial & Engineering Chemistry Research, 2014, 53, 17782-17793.	1.8	4
62	Entropy Flow and Energy Efficiency Analysis of Extractive Distillation with a Heavy Entrainer. Industrial & Engineering Chemistry Research, 2014, 53, 4778-4791.	1.8	29
63	Computer aided product design tool for sustainable product development. Computers and Chemical Engineering, 2014, 71, 362-376.	2.0	31
64	Extractive Distillation Process Optimisation of the 1.0-1a Class System, Acetone - methanol with Water. Computer Aided Chemical Engineering, 2014, 33, 1315-1320.	0.3	5
65	Extractive Distillation. , 2014, , 201-245.		12
66	Separation of ethyl acetateâ€“isooctane mixture by heteroazeotropic batch distillation. Chemical Engineering Research and Design, 2014, 92, 995-1004.	2.7	10
67	Generalised model for heteroazeotropic batch distillation with variable decanter hold-up. Separation and Purification Technology, 2013, 115, 9-19.	3.9	6
68	Modeling and simulation of melting curves and chemical interesterification of binary blends of vegetable oils. Chemical Engineering Science, 2013, 87, 14-22.	1.9	18
69	Extension of Thermodynamic Insights on Batch Extractive Distillation to Continuous Operation. 1. Azeotropic Mixtures with a Heavy Entrainer. Industrial & Engineering Chemistry Research, 2013, 52, 4606-4622.	1.8	56
70	Extension of Thermodynamic Insights on Batch Extractive Distillation to Continuous Operation. 2. Azeotropic Mixtures with a Light Entrainer. Industrial & Engineering Chemistry Research, 2013, 52, 4623-4637.	1.8	44
71	Thermodynamic Insights on the Feasibility of Homogeneous Batch Extractive Distillation. 3. Azeotropic Mixtures with Light Entrainer.. Industrial & Engineering Chemistry Research, 2012, 51, 4643-4660.	1.8	40
72	Thermodynamic Insights on the Feasibility of Homogeneous Batch Extractive Distillation. 4. Azeotropic Mixtures with Intermediate Boiling Entrainer. Industrial & Engineering Chemistry Research, 2012, 51, 6489-6501.	1.8	46

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73	AZEOTROPE PREDICTION BY MONTE CARLO MOLECULAR SIMULATION. Chemical Engineering Communications, 2012, 199, 673-688.	1.5	1
74	Comparison of predicted and experimental DSC curves for vegetable oils. Thermochimica Acta, 2012, 545, 96-102.	1.2	8
75	Operational and strategic alignment in the decision process of molecule substitution. Computer Aided Chemical Engineering, 2012, 30, 382-386.	0.3	1
76	Thermodynamic Efficiency and Cost-Effective Optimization of Heterogeneous Batch Distillation. Computer Aided Chemical Engineering, 2012, 30, 362-366.	0.3	4
77	Batch heteroazeotropic distillation with variable decanter hold-up. Computer Aided Chemical Engineering, 2012, 30, 527-531.	0.3	2
78	An integrated framework for product formulation by computer aided mixture design. Computer Aided Chemical Engineering, 2012, , 702-706.	0.3	7
79	Heterogeneous batch distillation with variable decanter hold-up. Computer Aided Chemical Engineering, 2012, 31, 1607-1611.	0.3	0
80	From batch to continuous extractive distillation using thermodynamic insight: Class 1.0–2 with a heavy entrainer. , 2011, , .		0
81	Optimization of Heterogeneous Batch Extractive Distillation. Industrial & Engineering Chemistry Research, 2011, 50, 5204-5217.	1.8	18
82	Phase Equilibrium and Optimization Tools: Application for Enhanced Structured Lipids for Foods. JAOCS, Journal of the American Oil Chemists' Society, 2011, 88, 223-233.	0.8	21
83	Prediction of miscible mixtures flash-point from UNIFAC group contribution methods. Fluid Phase Equilibria, 2011, 300, 70-82.	1.4	72
84	Multi-objective optimization of three-phase batch extractive distillation. Computer Aided Chemical Engineering, 2011, , 562-566.	0.3	10
85	Models driven conception of an Computer Aided Mixture Design tool. Computer Aided Chemical Engineering, 2011, 29, 1608-1612.	0.3	2
86	Optimisation of heterogeneous batch extractive distillation. Computer Aided Chemical Engineering, 2010, , 961-966.	0.3	2
87	Soft-SAFT modeling of vaporâ€“liquid equilibria of nitriles and their mixtures. Fluid Phase Equilibria, 2010, 289, 191-200.	1.4	13
88	Effect of stirring on the safety of flammable liquid mixtures. Journal of Hazardous Materials, 2010, 177, 1093-1101.	6.5	20
89	Flash Point for Ternary Partially Miscible Mixtures of Flammable Solvents. Journal of Chemical & Engineering Data, 2010, 55, 134-146.	1.0	42
90	Flash-Point Measurements and Modeling for Ternary Partially Miscible Aqueousâ^'Organic Mixtures. Journal of Chemical & Engineering Data, 2010, 55, 3451-3461.	1.0	31

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91	Computer-Aided Lipid Design: phase equilibrium modeling for product design. Computer Aided Chemical Engineering, 2010, 28, 271-276.	0.3	4
92	HIx system thermodynamic model for hydrogen production by the Sulfurâ€“Iodine cycle. International Journal of Hydrogen Energy, 2009, 34, 1696-1709.	3.8	20
93	Bunsen section thermodynamic model for hydrogen production by the sulfurâ€“iodine cycle. International Journal of Hydrogen Energy, 2009, 34, 6625-6635.	3.8	22
94	Effect of operating conditions and physicoâ€“chemical properties on the wet granulation kinetics in high shear mixer. Powder Technology, 2009, 190, 160-169.	2.1	96
95	Heterogeneous Batch Distillation Processes for Waste Solvent Recovery in Pharmaceutical Industry. Computer Aided Chemical Engineering, 2009, 27, 1119-1124.	0.3	4
96	Thermodynamic Insights on the Feasibility of Homogeneous Batch Extractive Distillation, 2. Low-Relative-Volatility Binary Mixtures with a Heavy Entrainer. Industrial & Engineering Chemistry Research, 2009, 48, 3560-3572.	1.8	39
97	How to Manage Complexity in Phase Equilibria Modeling? Application to the Bunsen Reaction. Computer Aided Chemical Engineering, 2009, , 333-338.	0.3	0
98	Thermodynamic Insights on the Feasibility of Homogeneous Batch Extractive Distillation, 1. Azeotropic Mixtures with a Heavy Entrainer. Industrial & Engineering Chemistry Research, 2009, 48, 3544-3559.	1.8	61
99	Solid-Liquid Equilibrium Modelling and Stability Tests for Triacylglycerols Mixtures. Computer Aided Chemical Engineering, 2009, 27, 885-890.	0.3	4
100	Optimized intermolecular potential for nitriles based on Anisotropic United Atoms model. Journal of Molecular Modeling, 2008, 14, 571-580.	0.8	5
101	Flash-point prediction for binary partially miscible mixtures of flammable solvents. Journal of Hazardous Materials, 2008, 153, 1165-1175.	6.5	59
102	Modeling the vaporâ€“liquid equilibrium and association of nitrogen dioxide/dinitrogen tetroxide and its mixtures with carbon dioxide. Fluid Phase Equilibria, 2008, 266, 154-163.	1.4	20
103	Heterogeneous batch distillation processes: Real system optimisation. Chemical Engineering and Processing: Process Intensification, 2008, 47, 408-419.	1.8	28
104	Computer aided aroma design Iâ€“Molecular knowledge framework. Chemical Engineering and Processing: Process Intensification, 2008, 47, 1902-1911.	1.8	18
105	Computer-aided aroma design. II. Quantitative structureâ€“odour relationship. Chemical Engineering and Processing: Process Intensification, 2008, 47, 1912-1925.	1.8	16
106	Flash-point prediction for binary partially miscible aqueousâ€“organic mixtures. Chemical Engineering Science, 2008, 63, 4543-4554.	1.9	46
107	Vapour reactive distillation process for hydrogen production by HI decomposition from HIâ€“I2â€“H2O solutions. Chemical Engineering and Processing: Process Intensification, 2008, 47, 396-407.	1.8	37
108	Heterogeneous extractive batch distillation of chloroformâ€“methanolâ€“water: Feasibility and experiments. Chemical Engineering Science, 2008, 63, 78-94.	1.9	29

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109	Modeling the phase equilibria of nitriles by the soft-SAFT Equation of State. Computer Aided Chemical Engineering, 2008, 25, 739-744.	0.3	3
110	Column configurations of continuous heterogeneous extractive distillation. AICHE Journal, 2007, 53, 1982-1993.	1.8	28
111	Separation of azeotropes in batch extractive stripper with intermediate entrainer. Computer Aided Chemical Engineering, 2006, 21, 793-797.	0.3	6
112	Multiclass molecular knowledge framework for product and process design. Computer Aided Chemical Engineering, 2006, 21, 889-894.	0.3	2
113	Practical residue curve map analysis applied to solvent recovery in non-ideal binary mixtures by batch distillation processes. Chemical Engineering and Processing: Process Intensification, 2006, 45, 672-683.	1.8	19
114	Quantitative structureâ€"Odor relationship: Using of multidimensional data analysis and neural network approaches. Computer Aided Chemical Engineering, 2006, 21, 895-900.	0.3	7
115	Heterogeneous batch distillation processes: Real system optimisation. Computer Aided Chemical Engineering, 2005, 20, 1081-1086.	0.3	0
116	Separation of n-hexaneâ€"ethyl acetate mixtures by azeotropic batch distillation with heterogeneous entrainers. Chemical Engineering and Processing: Process Intensification, 2005, 44, 131-137.	1.8	25
117	Feasibility study of heterogeneous batch extractive distillation. Computer Aided Chemical Engineering, 2005, , 895-900.	0.3	2
118	Modelling of a dynamic multiphase flash: the positive flash. Computers and Chemical Engineering, 2004, 28, 2469-2480.	2.0	1
119	Heterogeneous batch-extractive distillation of minimum boiling azeotropic mixtures. AICHE Journal, 2003, 49, 3074-3083.	1.8	40
120	The structure of the agrochemical fungicidal 4-chloro-3-(3,5-dichlorophenyl)-1H-pyrazole (RPA 406194) and related compounds. Tetrahedron, 2003, 59, 555-560.	1.0	20
121	Application of molecular simulation in the gibbs ensemble to predict liquid-vapor equilibrium curve of acetonitrile. Computer Aided Chemical Engineering, 2003, 14, 653-658.	0.3	2
122	Feasibility of heterogeneous batch distillation processes. AICHE Journal, 2002, 48, 1168-1178.	1.8	50
123	Analysis and Multiple Steady States of an Industrial Heterogeneous Azeotropic Distillation. Industrial & Engineering Chemistry Research, 2001, 40, 2914-2924.	1.8	16
124	Entrainer Selection Rules for the Separation of Azeotropic and Close-Boiling-Temperature Mixtures by Homogeneous Batch Distillation Process. Industrial & Engineering Chemistry Research, 2001, 40, 2729-2741.	1.8	62
125	Middle vessel heterogeneous batch distillation of an azeotropic mixture. Computer Aided Chemical Engineering, 2001, 9, 499-504.	0.3	2
126	Synthesis, experiments and simulation of heterogeneous batch distillation processes. Computers and Chemical Engineering, 2001, 25, 799-806.	2.0	30

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127	Mechanism of Calcite Crystal Growth Inhibition by the N-terminal Undecapeptide of Lithostathine. Journal of Biological Chemistry, 2000, 275, 1057-1064.	1.6	70
128	Synthesis, experiments and simulation of a heterogeneous batch distillation process. Computer Aided Chemical Engineering, 2000, , 1123-1128.	0.3	0
129	Nucleation studies of potassium hydrogen tartrate in model solutions and wines. Journal of Crystal Growth, 1996, 166, 172-178.	0.7	8
130	Molecular Modeling for Physical Property Prediction. , 0, , 107-135.		2