Carl I Steefel

List of Publications by Year
in descending order

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107 papers	8,915 citations	41323 49 h-index	42364 92 g-index
114 all docs	114 docs citations	114 times ranked	5918 citing authors

#	Article	IF	Citations
1	Reactive transport codes for subsurface environmental simulation. Computational Geosciences, 2015, 19, 445-478.	1.2	566
2	Reactive transport modeling: An essential tool and a new research approach for the Earth sciences. Earth and Planetary Science Letters, 2005, 240, 539-558.	1.8	546
3	A new kinetic approach to modeling water-rock interaction: The role of nucleation, precursors, and Ostwald ripening. Geochimica Et Cosmochimica Acta, 1990, 54, 2657-2677.	1.6	477
4	The role of reaction affinity and secondary minerals in regulating chemical weathering rates at the Santa Cruz Soil Chronosequence, California. Geochimica Et Cosmochimica Acta, 2009, 73, 2804-2831.	1.6	280
5	An investigation of the effect of pore scale flow on average geochemical reaction rates using direct numerical simulation. Water Resources Research, 2012, 48, .	1.7	238
6	The mineral dissolution rate conundrum: Insights from reactive transport modeling of U isotopes and pore fluid chemistry in marine sediments. Geochimica Et Cosmochimica Acta, 2006, 70, 337-363.	1.6	234
7	Molecular Dynamics Simulations of Water Structure and Diffusion in Silica Nanopores. Journal of Physical Chemistry C, 2012, 116, 11556-11564.	1.5	223
8	Acetate Availability and its Influence on Sustainable Bioremediation of Uranium-Contaminated Groundwater. Geomicrobiology Journal, 2011, 28, 519-539.	1.0	222
9	Expanding the role of reactive transport models in critical zone processes. Earth-Science Reviews, 2017, 165, 280-301.	4.0	207
10	Scale dependence of mineral dissolution rates within single pores and fractures. Geochimica Et Cosmochimica Acta, 2008, 72, 360-377.	1.6	199
11	Fluid-Rock Interaction: A Reactive Transport Approach. Reviews in Mineralogy and Geochemistry, 2009, 70, 485-532.	2.2	182
12	Pore-Scale Controls on Calcite Dissolution Rates from Flow-through Laboratory and Numerical Experiments. Environmental Science & Technology, 2014, 48, 7453-7460.	4.6	154
13	Diffusion and reaction in rock matrix bordering a hyperalkaline fluid-filled fracture. Geochimica Et Cosmochimica Acta, 1994, 58, 3595-3612.	1.6	153
14	Effects of physical and geochemical heterogeneities on mineral transformation and biomass accumulation during biostimulation experiments at Rifle, Colorado. Journal of Contaminant Hydrology, 2010, 112, 45-63.	1.6	137
15	Cesium migration in Hanford sediment: a multisite cation exchange model based on laboratory transport experiments. Journal of Contaminant Hydrology, 2003, 67, 219-246.	1.6	136
16	A reactive-transport model for weathering rind formation on basalt. Geochimica Et Cosmochimica Acta, 2011, 75, 7644-7667.	1.6	126
17	Chapter 2. APPROACHES TO MODELING OF REACTIVE TRANSPORT IN POROUS MEDIA. , 1996, , 83-130.		119
18	Multicomponent reactive transport in discrete fractures: I. Controls on reaction front geometry. Journal of Hydrology, 1998, 209, 186-199.	2.3	117

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19	Evolution of porosity and diffusivity associated with chemical weathering of a basalt clast. Journal of Geophysical Research, 2009, 114, .	3.3	117
20	The East River, Colorado, Watershed: A Mountainous Community Testbed for Improving Predictive Understanding of Multiscale Hydrologicalâ€“Biogeochemical Dynamics. Vadose Zone Journal, 2018, 17, 1-25.	1.3	115
21	Evaluation of mineral reactive surface area estimates for prediction of reactivity of a multi-mineral sediment. Geochimica Et Cosmochimica Acta, 2016, 188, 310-329.	1.6	108
22	Distinct Source Water Chemistry Shapes Contrasting Concentrationâ€Ðischarge Patterns. Water Resources Research, 2019, 55, 4233-4251.	1.7	103
23	Mineral Transformation and Biomass Accumulation Associated With Uranium Bioremediation at Rifle, Colorado. Environmental Science & Technology, 2009, 43, 5429-5435.	4.6	101
24	Water Table Dynamics and Biogeochemical Cycling in a Shallow, Variably-Saturated Floodplain. Environmental Science & Technology, 2017, 51, 3307-3317.	4.6	100
25	Upscaling calcium carbonate precipitation rates from pore to continuum scale. Chemical Geology, 2012, 318-319, 60-74.	1.4	99
26	Hot Spots and Hot Moments of Nitrogen in a Riparian Corridor. Water Resources Research, 2018, 54, 205-222.	1.7	99
27	Biostimulation induces syntrophic interactions that impact C, S and N cycling in a sediment microbial community. ISME Journal, 2013, 7, 800-816.	4.4	98
28	Measurement of accessible reactive surface area in a sandstone, with application to CO2 mineralization. Chemical Geology, 2012, 318-319, 113-125.	1.4	95
29	Micro-Continuum Approaches for Modeling Pore-Scale Geochemical Processes. Reviews in Mineralogy and Geochemistry, 2015, 80, 217-246.	2.2	88
30	Effect of fluid-sediment reaction on hydrothermal fluxes of major elements, eastern flank of the Juan de Fuca Ridge. Geochimica Et Cosmochimica Acta, 2002, 66, 1739-1757.	1.6	87
31	Pore Scale Processes Associated with Subsurface CO2 Injection and Sequestration. Reviews in Mineralogy and Geochemistry, 2013, 77, 259-303.	2.2	83
32	Physicochemical Heterogeneity Controls on Uranium Bioreduction Rates at the Field Scale. Environmental Science & Technology, 2011, 45, 9959-9966.	4.6	79
33	A 2.5D Reactive Transport Model for Fracture Alteration Simulation. Environmental Science & Technology, 2016, 50, 7564-7571.	4.6	79
34	Evaluation of accessible mineral surface areas for improved prediction of mineral reaction rates in porous media. Geochimica Et Cosmochimica Acta, 2017, 205, 31-49.	1.6	79
35	Pore-scale numerical investigation of the impacts of surface roughness: Upscaling of reaction rates in rough fractures. Geochimica Et Cosmochimica Acta, 2018, 239, 374-389.	1.6	79
36	Influence of hydrological, biogeochemical and temperature transients on subsurface carbon fluxes in a flood plain environment. Biogeochemistry, 2016, 127, 367-396.	1.7	76

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37	Simulation of mineral dissolution at the pore scale with evolving fluid-solid interfaces: review of approaches and benchmark problem set. Computational Geosciences, 2021, 25, 1285-1318.	1.2	72
38	A large column analog experiment of stable isotope variations during reactive transport: I. A comprehensive model of sulfur cycling and Î´34S fractionation. Geochimica Et Cosmochimica Acta, 2014, 124, 366-393.	1.6	71
39	Calcium isotope fractionation in groundwater: Molecular scale processes influencing field scale behavior. Geochimica Et Cosmochimica Acta, 2013, 119, 93-116.	1.6	70
40	Effects of pore-scale precipitation on permeability and flow. Advances in Water Resources, 2016, 95, 125-137.	1.7	70
41	Timing the Onset of Sulfate Reduction over Multiple Subsurface Acetate Amendments by Measurement and Modeling of Sulfur Isotope Fractionation. Environmental Science & Technology, 2012, 46, 8895-8902.	4.6	66
42	Geochemical Exports to River From the Intrameander Hyporheic Zone Under Transient Hydrologic Conditions: East River Mountainous Watershed, Colorado. Water Resources Research, 2018, 54, 8456-8477.	1.7	66
43	Reactive Transport in Evolving Porous Media. Reviews in Mineralogy and Geochemistry, 2019, 85, 197-238.	2.2	65
44	Implementation and evaluation of permeability-porosity and tortuosity-porosity relationships linked to mineral dissolution-precipitation. Computational Geosciences, 2015, 19, 655-671.	1.2	60
45	Reoxidation of Chromium(III) Products Formed under Different Biogeochemical Regimes. Environmental Science & Technology, 2017, 51, 4918-4927.	4.6	60
46	Surface Properties of Clay Minerals. Developments in Clay Science, 2015, 6, 5-31.	0.3	56
47	Exascale applications: skin in the game. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2020, 378, 20190056.	1.6	53
48	High-Resolution Simulation of Pore-Scale Reactive Transport Processes Associated with Carbon Sequestration. Computing in Science and Engineering, 2014, 16, 22-31.	1.2	51
49	Ionic Transport in Nano-Porous Clays with Consideration of Electrostatic Effects. Reviews in Mineralogy and Geochemistry, 2015, 80, 287-329.	2.2	51
50	Alteration and Erosion of Rock Matrix Bordering a Carbonate-Rich Shale Fracture. Environmental Science & Technology, 2017, 51, 8861-8868.	4.6	50
51	Mineralogical and transport controls on the evolution of porous media texture using direct numerical simulation. Water Resources Research, 2017, 53, 3645-3661.	1.7	49
52	Fracture Evolution in Multimineral Systems: The Role of Mineral Composition, Flow Rate, and Fracture Aperture Heterogeneity. ACS Earth and Space Chemistry, 2018, 2, 112-124.	1.2	49
53	Reactive Transport at the Crossroads. Reviews in Mineralogy and Geochemistry, 2019, 85, 1-26.	2.2	46
54	Benchmark reactive transport simulations of a column experiment in compacted bentonite with multispecies diffusion and explicit treatment of electrostatic effects. Computational Geosciences, 2015, 19, 535-550.	1.2	45

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55	A high resolution estimate of the inorganic nitrogen flux from the Scheldt estuary to the coastal North Sea during a nitrogen-limited algal bloom, spring 1995. Geochimica Et Cosmochimica Acta, 1999, 63, 1359-1374.	1.6	43
56	Benchmarks for multicomponent reactive transport across a cement/clay interface. Computational Geosciences, 2015, 19, 635-653.	1.2	43
57	Reactive Transport Modeling of Coupled Processes in Nanoporous Media. Reviews in Mineralogy and Geochemistry, 2019, 85, 75-109.	2.2	43
58	Upscaling Calcite Growth Rates from the Mesoscale to the Macroscale. Environmental Science & Technology, 2013, 47, 7555-7562.	4.6	42
59	Benchmarks for multicomponent diffusion and electrochemical migration. Computational Geosciences, 2015, 19, 523-533.	1.2	42
60	Assessing conceptual models for subsurface reactive transport of inorganic contaminants. Eos, 2004, 85, 449.	0.1	39
61	ParCrunchFlow: an efficient, parallel reactive transport simulation tool for physically and chemically heterogeneous saturated subsurface environments. Computational Geosciences, 2015, 19, 403-422.	1.2	39
62	Modeling Coupled Chemical and Isotopic Equilibration Rates. Procedia Earth and Planetary Science, 2014, 10, 208-217.	0.6	38
63	Fluid Flow, Heat Transfer, and Solute Transport at Nuclear Waste Storage Tanks in the Hanford Vadose Zone. Vadose Zone Journal, 2002, 1, 68-88.	1.3	35
64	Identifying geochemical hot moments and their controls on a contaminated river floodplain system using wavelet and entropy approaches. Environmental Modelling and Software, 2016, 85, 27-41.	1.9	35
65	Feedbacks Between Hydrological Heterogeneity and Bioremediation Induced Biogeochemical Transformations. Environmental Science & Technology, 2009, 43, 5197-5204.	4.6	34
66	Complete Restriction of ³⁶Cl^{â€“} Diffusion by Celestite Precipitation in Densely Compacted Illite. Environmental Science and Technology Letters, 2015, 2, 139-143.	3.9	34
67	Geochemical Kinetics and Transport. , 2008, , 545-589.		33
68	Multi-scale Model of Reactive Transport in Fractured Media: Diffusion Limitations on Rates. Transport in Porous Media, 2019, 128, 701-721.	1.2	32
69	Reactive transport benchmarks for subsurface environmental simulation. Computational Geosciences, 2015, 19, 439-443.	1.2	31
70	A reactive transport benchmark on heavy metal cycling in lake sediments. Computational Geosciences, 2015, 19, 613-633.	1.2	30
71	Hysteresis Patterns of Watershed Nitrogen Retention and Loss Over the Past 50Âyears in United States Hydrological Basins. Global Biogeochemical Cycles, 2021, 35, e2020GB006777.	1.9	29
72	Benchmarking the simulation of Cr isotope fractionation. Computational Geosciences, 2015, 19, 497-521.	1.2	27

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73	Benchmark problems for reactive transport modeling of the generation and attenuation of acid rock drainage. Computational Geosciences, 2015, 19, 599-611.	1.2	26
74	Incorporating Nanoscale Effects into a Continuum-Scale Reactive Transport Model for CO₂-Deteriorated Cement. Environmental Science & Technology, 2017, 51, 10861-10871.	4.6	25
75	Modeling the Ionic Strength Effect on Diffusion in Clay. The DR-A Experiment at Mont Terri. ACS Earth and Space Chemistry, 2019, 3, 442-451.	1.2	25
76	Divergent Aquifer Biogeochemical Systems Converge on Similar and Unexpected Cr(VI) Reduction Products. Environmental Science & Technology, 2014, 48, 10699-10706.	4.6	24
77	Sequential Imputation of Missing Spatio-Temporal Precipitation Data Using Random Forests. Frontiers in Water, 2020, 2, .	1.0	24
78	Differential C-Q Analysis: A New Approach to Inferring Lateral Transport and Hydrologic Transients Within Multiple Reaches of a Mountainous Headwater Catchment. Frontiers in Water, 2020, 2, .	1.0	24
79	Chemical affinity and pH effects on chlorite dissolution kinetics under geological CO2 sequestration related conditions. Chemical Geology, 2015, 396, 208-217.	1.4	23
80	Solid phase evolution in the Biosphere 2 hillslope experiment as predicted by modeling of hydrologic and geochemical fluxes. Hydrology and Earth System Sciences, 2009, 13, 2273-2286.	1.9	23
81	Strontium and Cesium Release Mechanisms during Unsaturated Flow through Waste-Weathered Hanford Sediments. Environmental Science & Technology, 2011, 45, 8313-8320.	4.6	21
82	Investigating calcite growth rates using a quartz crystal microbalance with dissipation (QCM-D). Geochimica Et Cosmochimica Acta, 2018, 222, 269-283.	1.6	19
83	A Poreâ€Scale Investigation of Mineral Precipitation Driven Diffusivity Change at the Columnâ€Scale. Water Resources Research, 2021, 57, e2020WR028483.	1.7	19
84	Early Diagenesis of Lacustrine Carbonates in Volcanic Settings: The Role of Magmatic CO₂ (Lake Dziani Dzaha, Mayotte, Indian Ocean). ACS Earth and Space Chemistry, 2020, 4, 363-378.	1.2	18
85	Modeling diffusion processes in the presence of a diffuse layer at charged mineral surfaces: a benchmark exercise. Computational Geosciences, 2021, 25, 1319-1336.	1.2	17
86	Determining How Critical Zone Structure Constrains Hydrogeochemical Behavior of Watersheds: Learning From an Elevation Gradient in California's Sierra Nevada. Frontiers in Water, 2020, 2, .	1.0	17
87	Modeling the Impact of Riparian Hollows on River Corridor Nitrogen Exports. Frontiers in Water, 2021, 3, .	1.0	15
88	Wavelet-based local mesh refinement for rainfallâ€“runoff simulations. Journal of Hydroinformatics, 2020, 22, 1059-1077.	1.1	14
89	Rates and mechanisms of uranyl oxyhydroxide mineral dissolution. Geochimica Et Cosmochimica Acta, 2017, 207, 298-321.	1.6	12
90	Investigation of Coupled Processes in Fractures and the Bordering Matrix via a Microâ€Continuum Reactive Transport Model. Water Resources Research, 2022, 58, .	1.7	12

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91	From legacy contamination to watershed systems science: a review of scientific insights and technologies developed through DOE-supported research in water and energy security. Environmental Research Letters, 2022, 17, 043004.	2.2	12
92	Dissolved Carbonate and pH Control the Dissolution of Uranyl Phosphate Minerals in Flow-Through Porous Media. Environmental Science & Technology, 2020, 54, 6031-6042.	4.6	11
93	Solving the Nernstâ€Planck Equation in Heterogeneous Porous Media With Finite Volume Methods: Averaging Approaches at Interfaces. Water Resources Research, 2020, 56, e2019WR026832.	1.7	11
94	A model for discrete fracture-clay rock interaction incorporating electrostatic effects on transport. Computational Geosciences, 2021, 25, 395-410.	1.2	9
95	Modeling geogenic and atmospheric nitrogen through the East River Watershed, Colorado Rocky Mountains. PLoS ONE, 2021, 16, e0247907.	1.1	9
96	Hot Spots and Hot Moments in the Critical Zone: Identification of and Incorporation into Reactive Transport Models. , 2022, , 9-47.		7
97	Secondary magnesite formation from forsterite under CO2 sequestration conditions via coupled heterogeneous nucleation and crystal growth. Geochimica Et Cosmochimica Acta, 2021, 311, 29-42.	1.6	6
98	Microscale Mechanicalâ€Chemical Modeling of Granular Salt: Insights for Creep. Journal of Geophysical Research: Solid Earth, 2021, 126, .	1.4	6
99	Microbially mediated kinetic sulfur isotope fractionation: reactive transport modeling benchmark. Computational Geosciences, 2021, 25, 1379-1391.	1.2	5
100	Fluid Flow, Heat Transfer, and Solute Transport at Nuclear Waste Storage Tanks in the Hanford Vadose Zone. Vadose Zone Journal, 2002, 1, 68.	1.3	5
101	7. Micro-Continuum Approaches for Modeling Pore-Scale Geochemical Processes. , 2015, , 217-246.		2
102	Fluid Flow, Heat Transfer, and Solute Transport at Nuclear Waste Storage Tanks in the Hanford Vadose Zone. Vadose Zone Journal, 2002, 1, 68-88.	1.3	2
103	7. Reactive Transport in Evolving Porous Media. , 2019, , 197-238.		1
104	1. Reactive Transport at the Crossroads. , 2019, , 1-26.		0
105	4. Reactive Transport Modeling of Coupled Processes in Nanoporous Media. , 2019, , 75-110.		0
106	Guest Editorial to the CouFrac 2018 Special Issue Coupled Thermal-Hydro-Mechanical-Chemical Processes in Fractured Media: Microscale to Macroscale Numerical Modeling. Computational Geosciences, 2020, 24, 1747-1749.	1.2	0
107	Editorial: Chemical Export to River Systems From the Critical Zone. Frontiers in Water, 2022, 3, .	1.0	0