



Curriculum Vitae for *CARL I. STEEFEL*

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EDUCATION:

1992 Yale University - Ph.D Geochemistry
1987 Yale University - M.Phil. Geology
1982 University of Colorado, Boulder - M.S. Geology.
1974 Washington University - B.A. English Literature
1972 Princeton University

EXPERIENCE:

2016-Present Department Head, Geochemistry, Earth and Environmental Sciences Area
2012-Present Senior Scientist, Lawrence Berkeley National Lab
2004-2012 Staff Scientist, Lawrence Berkeley National Lab
1998-2004 Staff Scientist, Environmental Science Division, Lawrence Livermore National Laboratory
1995-1998 Assistant Professor of Geology, University of South Florida
1995 Senior Research Scientist, Interfacial Geochemistry Group, Battelle Pacific Northwest Laboratories
1993-1995 Research Scientist, Interfacial Geochemistry Group, Battelle Pacific Northwest Laboratories
1991-1992 Post-Doctoral Associate, Mineralogisch-Petrographisches Institut, Universitat Bern, Switzerland
1985-1991 Teaching and research fellowships, Yale University Department of Geology
1979-1985 Geologist, Anaconda Minerals
1978 Geological Assistant, USGS Branch of Exploration Research
1976 Manuscripts librarian, Huntington Library, San Marino, California

RESEARCH INTERESTS:

High performance computing: HPC modeling of integrated terrestrial water and nutrients, subsurface fracture evolution
Machine learning: Hybrid and reduced dimension/order models for watershed biogeochemical function
Reactive transport modeling: Numerical modeling of pore scale processes, reactive contaminant transport, reactive transport in clays, chemical weathering and negative emissions of CO₂
Mineral-water kinetics: Mineral dissolution and precipitation kinetics
Biogeochemistry: Biogeochemical reactions in groundwater, estuaries, and oceans

AWARDS & RECOGNITION:

- 2020 Berkeley Lab Director's Award for Exceptional Scientific Achievement
- 2019 American Geophysical Union Fellow
- 2017 R&D 100 Award Winner for reactive transport software CrunchFlow (<https://www.rd100conference.com/awards/winners-finalists/year/2017/>)
- 2007 Award for outstanding contributions to basic research in the geosciences, Geosciences Research Program, Division of Chemical Sciences, Geosciences, and Biosciences, U.S. Department of Energy, May 2007.
- 1990 Philip M. Orville Prize for outstanding research and scholarship, Dept. of Geology and Geophysics, Yale University
- 1990 Best Student Contribution, 2nd International Symposium on the Geochemistry of the Earth's Surface and of Mineral Formation, Aix-en-Provence, France
- 1989 Outstanding Mention, GSA Research Proposal
- 1974 Phi Beta Kappa, Washington University

CURRENT PROJECT LEADERSHIP

- Lead PI, Subsurface Exascale Computing Project (DOE: 6 years, ~\$18M)
- Lead PI, ExaSheds Project (DOE BER: 4 years, ~\$8.3M)
- Deputy Director, *Nanoscale Control of Geologic CO₂* Energy Frontier Research Center (DOE BES: 8 years, ~\$15M)
- Co-PI and Component Lead, Watershed Function Science Focus Area (3 years, \$21M)
- Component Lead, Discovery Geosciences for DOE Basic Energy Science

MENTORSHIP & SUPERVISION

Supervision of approximately 20 early career staff over 20 years, and mentoring of hundreds of early career reactive transport modeling through collaborations and 17 short courses.

PROFESSIONAL SERVICE & ACTIVITIES (SELECT):

Editorships:

- Specialty Chief Editor, Water and the Critical Zone, *Frontiers in Water*, 2018-present
- Associate Editor, *Geochimica et Cosmochimica Acta*, June 2011-present
- Lead Editor, *Reviews in Mineralogy and Geochemistry* **80** "Pore-Scale Geochemical Processes" 2015.
- Co-Editor, *Reviews in Mineralogy* **34**, "Reactive Transport in Porous Media", 1996.
- Lead Editor of a Special Issue of *Computational Geoscience* on Subsurface Environmental Benchmark Modeling
- *Journal of Contaminant Hydrology*, Associate Editor 2005-present
- *Journal of Hydrology*, Associate Editor (2002-2007)
- *American Journal of Science*, Associate Editor (2002-2004)

Workshop / Committee / Advisory Leadership:

- Workshop Co-Organizer, Reactive Transport for the Earth and Environmental Sciences in the 21st Century, Clos Lucé, Amboise, France, October 2-4, 2017.
- Lead organizer and editor: *Reviews in Mineralogy and Geochemistry* short course and volume on "Pore Scale Geochemical Processes", 2015
- Chair: International benchmarking for reactive transport working group, 2012-2018

- Panelist 2011 Goldschmidt theme *Frontiers in Computational Geochemistry*.
- Co-chair for 2009 Goldschmidt Theme *Frontiers in Computational Geochemistry*.
- Review Panel: state of flow and transport modeling at the Hanford Site, November 2005.
- Yucca Mountain Unsaturated Zone/Radionuclide Transport Model Peer Review Panel, member, January-July, 1999.

Instructor

- Developer and instructor: 17 short courses in reactive transport modeling
- Co-instructor: Graduate level course in “Numerical Modeling in the Earth and Environmental Sciences”, UC Berkeley, Spring 2019.
- Lead Instructor, CrunchTope Short Course at CouFrac Conference, Wuhan, China, November 10-11, 2018.
- Lead Instructor, CrunchTope Short Course at “Reactive Transport for the Earth and Environmental Sciences in the 21st Century” workshop in Amboise, France, October 5, 2017
- Lead Instructor, CrunchTope Short Course, Pohang University of Technology, Pohang, South Korea, December 6-8, 2016.
- Lead instructor for short course in Reactive Transport Modeling: University of Bern (4 times), Bureau de Recherches Géologiques et Minières, LBNL, Penn State, Shell Oil, Heriot-Watt University, University of Minnesota
- Lead Instructor, CrunchTope Short Course, 2016 Goldschmidt Conference, June 25-26, 2016.
- Lead Instructor, CrunchTope Short Course, University of Illinois, June 8-9, 2016.
- Lead Instructor, CrunchFlow Short Course, March 22-23, 2016, Imperial College, London.
- Lead Instructor, CrunchFlow Short Course, August 24-25, 2013 Goldschmidt Conference, Florence, Italy.

Other:

- Principal developer of CrunchFlow Reactive Transport software package
- Member: American Geophysical Union, Geochemical Society

KEYNOTE AND INVITED PRESENTATIONS:

- 2020 Keynote Address “Data-Intensive Models for Pore to Plume to Watershed Scales”, Goldschmidt 2020, Oahu, Hawaii.
- 2020 Keynote Address “Reactive Transport at the Crossroads: Progress and New Directions”, “How to integrate geochemistry at affordable costs into reactive transport for large-scale systems”, 5 - 7 February 2020, Helmholtz-Zentrum Dresden-Rossendorf, Germany.
- 2019 Invited Address “Modeling Reactive Transport in Clay Fractures”, with C. Tournassat, 2019 AGU Meeting
- 2019 Keynote address, “Reactive Transport at the Crossroads”, P. Van Cappellen Festschrift Workshop, University of Waterloo, Canada.
- 2019 Keynote address, “CrunchClay: A Mean Electrostatic Potential Model for Ion Transport in Clay”, EuroClay 2019, July 5, 2019, Paris, France.
- 2019 Invited Address “Reactive Transport at the Crossroads”, Panel Review and Workshop for the TPC Project Taiwan, Taipei, Taiwan, June 26, 2019
- 2018 Keynote Address “Crossing Scales in Porous Media”, Tough Symposium, Berkeley, CA, October 10, 2018.
- 2018 Keynote Address “Modeling Chemical and Mechanical Effects in Fractures”, CouFrac Conference, Wuhan, China, November 12, 2018
- 2018 Keynote Address “Interpreting Laboratory and Field Geochemical Systems with Reactive Transport Modeling”, 2018 Goldschmidt Conference, August 15, 2018, Boston.

- 2017 Keynote Address “A Mean Electrostatic Model for Ion Transport through Heterogeneous Clay”, 2017 Clay Conference, Davos, Switzerland, September 27, 2017.
- 2017 Keynote Address “Reactive Transport at the Crossroads”, Workshop on *Reactive Transport for the Earth and Environmental Sciences in the 21st Century*, Clos Lucé, Amboise, France, October 2, 2017.
- 2017 “The Lab-Field Rate Discrepancy Revisited”, Invited talk at Susan Brantley 2017 Geochemistry Medal session, American Chemical Society, April 4, 2017.
- 2016 “Multi-Scale Reactive Transport Modeling,” Workshop at Bureau de Recherches Géologiques et Minières, Orleans, France, October 25, 2016
- 2016 “Multi-scale reactive transport modeling of terrestrial systems,” Plenary Invited Talk, EPSRC Workshop on *Reactive Transport in Porous Media*, Imperial College London.
- 2016 “New Approaches to Modeling Water-Rock-Gas Interaction,” Invited Talk at Cambridge University, UK, March 24, 2016
- 2016 “Reactive transport modeling for evaluation and optimization of architected materials,” with C. Tournassat, Keynote Talk at 2016 Goldschmidt
- 2016 “A New Approach to Modeling Nucleation, Crystal Growth, and the Ostwald Step Rule,” Invited Talk at Spring 2016 American Chemical Society Meeting, San Diego, CA
- 2015 “Multiple Scale (and Multi-Scale) Reactive Transport Modeling of Terrestrial Systems,” Keynote Address at 2015 Goldschmidt in Prague, Czech Republic, Aug. 20, 2015.
- 2015 “Contaminant Fate and Transport in Geological Environments,” Keynote address at Basic Research Needs workshop for Environmental Management, Bethesda, MD, 8 July, 2015.
- 2015 “Modeling Reactive Transport in Fractured Shales,” Invited Talk at the *Shale at all Scales* Workshop, Santa Fe, NM, 10 June, 2015.
- 2014 “The GEWaSC Framework: Multiscale Modeling of Coupled Biogeochemical, Microbiological, and Hydrological Processes,” Invited Talk at 2014 Goldschmidt Conference, Sacramento, CA, June 13, 2014
- 2014 “What is the State of the Art in Reactive Transport Modeling,” presented at an NSF workshop on Expanding the role of Reactive Transport Modeling (RTM) within the Biogeochemical Sciences, Arlington, VA, April 14, 2014
- 2014 “Genome-Enabled Watershed Simulation Capability (GEWaSC),” Plenary Talk at Terrestrial Ecosystem and Subsurface Biogeochemical Research meeting, Potomac, MD, May 6, 2014
- 2014 “Reactive Transport Models (RTM): Pores to Plots to Watersheds” presented at DOE Workshop on Computational Challenges for Mechanistic Modeling of Terrestrial Environments, Gaithersburg, MD, March 26, 2014.
- 2013 “What are the Time Scales for Carbonate Mineral Sequestration in the Subsurface?” presented at the 2013 Fall American Geophysical Union meeting, San Francisco, CA, Dec. 11, 2013.
- 2013 “Intercomparison of Reactive Transport Models” at 2013 SIAM meeting, Padova, Italy, June 19, 2013.
- 2013 “Approaches for Assessing Time Scales for Carbonate Mineral Sequestration” at Helmholtz-Zentrum für Umweltforschung (UFZ), Potsdam, Germany, May 13, 2013.
- 2013 “Reaction Fronts: Microscopic and Macroscopic” at Kongsberg Seminar, Kongsberg, Norway, May 9, 2013.
- 2013 “Time Scales for Carbonate Mineral Sequestration” at Washington University, May 1, 2013.
- 2013 “What are the time Scales for Carbonate Mineral Sequestration of CO₂ in the Subsurface,” Yale University Department of Geology, February 14, 2013.
- 2013 “Experimental and Modeling Studies to Determine Time Scales for Carbonate Mineral Sequestration” at Le Studium Conference, Orleans, France, February 25, 2013.
- 2012 “Pore to Flood Plain Scale Modeling of Reactive Transport” at 2012 Fall AGU Meeting, San Francisco, Ca, December 4, 2012.

- 2012 “Characterization and Modeling of Reactivity in a Sandstone containing Internal Diffusion-Controlled Zones” at BES Geosciences Workshop on Reaction and Transport within Internal Domains of Porous Medium, December 2, 2012.
- 2012 “What are the time Scales for Carbonate Mineral Sequestration of CO₂ in the Subsurface,” Colorado School of Mines, November 15, 2012.
- 2012 “What are the time Scales for Carbonate Mineral Sequestration of CO₂ in the Subsurface,” University of Missouri, Kansas City, November 7, 2012.
- 2012 “New Directions in Reactive Transport Modeling” at Subsurface Simulation Benchmark Workshop, National Central University, Taiwan, November 29, 2012.
- 2012 “What are the time Scales for Carbonate Mineral Sequestration of CO₂ in the Subsurface,” UCLA Department of Earth and Planetary Sciences, October 4, 2012.
- 2012 “Diffusion versus Surface Reaction Control of Mineral Precipitation and Dissolution Kinetics at the Pore Scale” at Goldschmidt 2012, Montreal, Canada, June 27, 2012.
- 2011 Invited speaker, Upscaling Carbonate Precipitation Associated with CO₂ Sequestration, American Geophysical Union Fall Meeting
- 2011 Invited speaker, Pore Scale Modeling of Mixing-Induced Carbonate Precipitation, American Geophysical Union Fall Meeting
- 2011 Keynote speaker, American Chemical Society Symposium *Multiscale Spatiotemporal Complexity in Geologic Carbon Sequestration: Linking Experimentation and Modeling*, August 2011.
- 2011 Invited speaker, Stanford University Geochemistry Colloquium.
- 2011 Invited speaker at Geochemical Transport in Compacted Clays, Bern, Switzerland.
- 2011 Invited speaker at workshop on Glass Corrosion, Manchester, England.
- 2010 Invited speaker, American Geophysical Union symposium *CO₂ Sequestration Inside Pores: From Molecules to Microbes*, December, 2010.
- 2010 Invited speaker at Department of Geological Sciences, University of Oregon.
- 2009 Invited speaker, Modeling Waste Form Performance in the Near-Field Environment, *Waste Form Performance and Technology*, U.S. National Academy of Sciences, November 4, 2009.
- 2008 Keynote speaker, 2008 Goldschmidt Conference, *Modeling of Thermodynamic and Kinetic Controls on Complex Biogeochemical Reaction Networks*.
- 2007 Keynote speaker, 2007 Goldschmidt Conference, *Interpreting Reaction Rates at the Field Scale*.
- 2006 Keynote speaker, American Chemical Society Symposium *Understanding Radionuclide Transport in the Environment: Remediation, Nuclear Waste Disposal, and Long-Term Stewardship*, March 2007.
- 2005 Keynote speaker, Geochemical and Transport Modeling, *10th International Conference on Migration of Behaviour of Actinides and Fission Products in the Geosphere*, Migration 2005 Avignon, France, September, 2005.
- 2005 Invited speaker, Conceptualizing Subsurface Biogeochemical Processes, *2005 International Symposium for Subsurface Microbiology, Jackson, Wyoming, August, 2005*.
- 2004 Invited speaker, Quantifying Rates in Biogeochemical Reaction Networks, *2004 Goldschmidt Conference*, June 2004.
- 2004 Keynote speaker, Reactive transport modeling of multicomponent cation exchange at the laboratory and field scale, *Workshop on Conceptual Model Development for Subsurface Reactive Transport Modeling of Inorganic Contaminants, Radionuclides, and Nutrients*, April 20-22, 2004, Albuquerque, New Mexico.
- 2003 Keynote speaker, *International Conference on Gas-Water-Rock Interaction with Application to CO₂ Sequestration and Petroleum Migration*, Institut Francaise du Petrole, Rueuil-Malmaison, France, Nov. 20-22, 2003.
- 2001 Invited speaker, DOE NABIR Workshop on Biogeochemical Modeling, October 21-22, 2001 at Pennsylvania State University.

- 2001 Invited speaker, 2001 Goldschmidt Meeting, Session on *Metals in the Weathering Environment*
- 2000 Plenary session speaker, *Computational Methods in Water Resources XIII*, June 25-29, 2000, Calgary, Canada.
- 2001 Invited speaker, AGU special session *Coupled Biogeochemical Processes Affecting the Transport of Contaminants in the Subsurface*, spring 2000
- 1999 University of Waterloo, Waterloo, Canada, a seminar entitled *Comparing Laboratory and Field Reaction/Weathering Rates: Is There a Discrepancy*, April 27, 1999.
- 1999 Woods Hole Oceanographic Institute, a seminar on *Reactive Transport in Discrete Fractures: The role of Chemical Kinetics and Permeability Change*, April 15, 1999.
- 1999 University of Oregon Department of Geology, a seminar on *Reactive Transport in Discrete Fractures: A Case Study from Maqarin, Jordan*, March 12, Eugene, Oregon.
- 1999 Oregon State University Department of Geology, a seminar on *Reactive Transport in Discrete Fractures: A Case Study from Maqarin, Jordan*, March 11, Corvallis, Oregon.
- 1998 *Geochemical Kinetics: From the Laboratory to the Field*, presented at the European Research Conference on *Geochemistry of Crustal Fluids: Characterization of Reactive Transport in Natural Systems*. May 22-27, Heraklion, Crete.
- 1997 *Overview of Modeling of Coupled Reactive Transport Processes* presented at the Alternative Models and Interpretations for the Near-Field Altered Zone Coupled Effects Expert Elicitation Workshop, Dec. 3-4, 1997, Las Vegas, Nevada.
- 1997 *Incorporating Intra-Aqueous Kinetics into Reactive Transport Models* presented at a Workshop on Modeling Reactive Transport held at Battelle PNNL, Nov. 28-Dec.2, 1997.
- 1996 Geological Society of America Symposium on *Application of Reactive Transport Modeling to Natural Systems*, October 28.
- 1996 Approaches to Modeling Reactive Transport, presented at the Mineralogical Society of America Short Course on *Reactive Transport in Porous Media*, October 25-27, Golden, Colorado.
- 1995 Keynote Speaker, European Research Conference on *Natural Waters and Water Technologies*, November 3-8, Lenggries, Germany.
- 1995 Departmental colloquium, University of Idaho, March 10, Moscow, Idaho.
- 1994 Keynote Speaker, Chapman Conference on "Hydrogeologic Processes: Building and Testing Atomistic to Basin-Scale Models," June 6-9, 1994, Lincoln, New Hampshire

PUBLICATIONS:

Google Scholar for Carl Steefel:

<https://scholar.google.com/citations?user=Yv-KZG0AAAAJ&hl=en>

ResearcherID for Carl Steefel:

<http://www.researcherid.com/rid/B-7758-2010>

Articles

- Hu, M., Rutqvist, J., **Steefel, C.** (2021) Mesh generation and optimization from digital rock fractures based on neural style transfer. *Journal of Rock Mechanics and Geotechnical Engineering*.
- Birkholzer JT, J Morris, JR Bargar, F Brondolo, A Cihan, D Crandall, H Deng, W Fan, W Fu, P Fu, A Hakala, Y Hao, J Huang, AD Jew, T Kneafsey, Z Li, C Lopano, J Moore, G Moridis, S Nakagawa, V Noël, M Reagan, CS Sherman, R Settgest, **C Steefel**, M Voltolini, W Xiong, J Ciezobka (2021) A New Modeling Framework for Multi-Scale Simulation of Hydraulic Fracturing and Production from Unconventional Reservoirs. *Energies* **14** (3): 641.

- Yan, Q., Wainwright, H., Dafflon, B., Uhlemann, S., **Steeffel, C.I.**, Falco, N., Kwang, J. and Hubbard, S.S., 2021. Hybrid data-model-based mapping of soil thickness in a mountainous watershed. *Earth Surface Dynamics Discussions*: 1-23.
- Newcomer, Michelle, Nicholas J. Bouskill, Haruko Wainwright, Taylor Maavara, Bhavna Arora, Erica R. Siirila-Woodburn, Dipankar Dwivedi, Ken Williams, **Carl Steefel**, and Susan S. Hubbard. (2020) Hysteresis Patterns of Watershed Nitrogen Retention and Loss over the past 50 years in United States Hydrological Basins. *Earth and Space Science Open Archive*, 10.1002/essoar.10504643.1.
- Liu X, Tournassat, C and **Steeffel CI** (2020) Preface to Multiscale Simulation in Geochemistry. *Geochimica et Cosmochimica Acta* **291**: 1-4.
- Hu, M., **Steeffel CI** and Rutqvist, J (2020) Guest Editorial to the CouFrac 2018 Special Issue Coupled Thermal-Hydro-Mechanical-Chemical Processes in Fractured Media: Microscale to Macroscale Numerical Modeling. *Computational Geosciences*: 1-3.
- Steeffel, C.I.** and C. Tournassat (2020) A model for discrete fracture-clay rock interaction incorporating electrostatic effects on transport. *Computational Geosciences* **25 (1)**: 395-410. DOI: 10.1007/s10596-020-10012-3.
- Ackerer J, **Steeffel C**, Liu F, Bart R, Safeeq M, O'Geen A, Hunsaker C and Bales R (2020) Determining how Critical Zone structure constrains hydrogeochemical behavior of watersheds: Learning from an elevation gradient in California's Sierra Nevada. *Frontiers in Water* **2**:23. DOI: 10.3389/frwa.2020.0002
- Arora B, Burrus M, Newcomer M, **Steeffel C**, Carroll RWH, Dwivedi D, Dong W, Williams K and Hubbard S (2020) Differential C-Q analysis: A new approach to inferring lateral transport and hydrologic transients within multiple reaches of a mountainous headwater catchment. *Frontiers of Water* **2**:24. DOI: 10.3389/frwa.2020.00024
- Mital, U, D. Dwivedi, J.B. Brown, B. Faybishenko, S.L. Painter, **C.I. Steefel** (2020) Sequential imputation of missing spatio-temporal precipitation data using Random Forests. *Frontiers in Water* **2**: 20. doi: 10.3389/frwa
- Cheng, Y., B. Arora, S. Sengor, J. Druhan, C. Wanner, B. M. van Breukelen, and **C. I. Steefel** (2020), Microbially mediated kinetic sulfur isotope fractionation: Reactive transport modeling benchmark, *Computational Geoscience* DOI: 10.1007/s10596-020-09988-9.
- Arora, B., M.S. Briggs, J. Zarnetske, J. Stegen, J. Gomez-Valez, D. Dwivedi, **C. I. Steefel** (2020) Hot spots and hot moments in the Critical Zone: Identification of and incorporation into reactive transport models. Springer Nature. J. Chorover (ed.)
- Reinoso-Maset, Estela, Perdrial, Nicolas, **Steeffel, Carl**, Um, Wooyong, Chorover, Jon, O'Day, Peggy (2020) Dissolved carbonate and pH control the dissolution of uranyl phosphate minerals in flow-through porous media. *Environmental Science and Technology*. <https://DOI.org/10.1021/acs.est.9b06448>
- Özgen-Xian, I., G. Kesserwani, D. Caviedes-Voullième, S. Molins, Z. Xu, D. Dwivedi, J. D. Moulton, and **C. I. Steefel** (2020) Wavelet-based local mesh refinement for rainfall-runoff simulations. *Journal of Hydroinformatics*. <https://DOI.org/10.2166/hydro.2020.198>
- Tournassat, C., **C. Steefel**, T. Gimmi (2020) Solving the Nernst-Planck equation in heterogeneous porous media with finite volume methods: Averaging approaches at interfaces. *Water Resources Research* <https://DOI.org/10.1029/2019WR026832>.
- Milesi, V.P., M. Debure, N.C.M Marty, M. Capano, D. Jézéquel, **C. Steefel**, ..., M. Ader (2020) Early diagenesis of lacustrine carbonates in volcanic settings: The role of magmatic CO₂ (Lake Dziani Dzaha, Mayotte, Indian Ocean). *Earth and Space Chemistry*. <https://dx.DOI.org/10.1021/acsearthspacechem.9b00279>.
- Alexander, F., A. Almgren, ... D.B. Kothe, ... **C.I. Steefel**, ... (2020) Exascale applications: skin in the game, *Philosophical Transactions of the Royal Society A* **378** (2166), 20190056.
- Molins, S., Soulaïne, C., Prasianakis, N.I., ..., **C.I. Steefel** (2020). Simulation of mineral dissolution at the pore scale with evolving fluid-solid interfaces: review of approaches and

benchmark problem set. *Computational Geosciences*. <https://DOI.org/10.1007/s10596-019-09903-x>

- Maina, F.Z., E. Siriila-Woodburn, M. Newcomer, C.I. Steefel (2020) Determining the impact of a severe dry to wet transition on watershed hydrodynamics in California, USA with an integrated hydrologic model. *J. Hydrology* **580**: <https://DOI.org/10.1016/j.jhydrol.2019.124358>
- Tournassat, C.M., Steefel, C.I. (2019) Modeling diffusion processes in the presence of a diffuse layer at charged mineral surfaces. A benchmark exercise. *Computational Geosciences*. 1-18. <https://DOI.org/10.1007/s10596-019-09845-4>.
- Steefel, C.I. (2019) Reactive transport at the crossroads. *Reviews in Mineralogy and Geochemistry* **85**: 1-26.
- Seigneur, N., Mayer, K.U., Steefel, C.I. (2019) Reactive transport of evolving porous media. *Reviews in Mineralogy and Geochemistry* **85**: 197-238.
- Tournassat, C.M., Steefel, C.I. (2019) Reactive transport modeling of coupled processes in nanoporous media. *Reviews in Mineralogy and Geochemistry* **85**: 75-109.
- Zhi, W., L. Li, W. Dong, W. Brown, J. Kaye, C.I. Steefel, K.H. Williams (2019) Distinct source water chemistry shapes contrasting concentration-discharge patterns. *Water Resources Research* **55**: 4233-4251. [10.1029/2018WR024527](https://doi.org/10.1029/2018WR024527).
- Molins, S., Trebotich, D., Arora, B., Steefel, C. I., & Deng, H. (2019) Multi-scale model of reactive transport in fractured media: Diffusion limitations on rates. *Transport in Porous Media* **128** (2): 701-721.
- Soler, J. M., Steefel, C. I., Gimmi, T., Leupin, O. X., & Cloet, V. (2019). Modeling the ionic strength effect on diffusion in clay. The DR-A experiment at Mont Terri. *ACS Earth and Space Chemistry* **3**: 442-451.
- Susan S. Hubbard, Kenneth Hurst Williams, Deb Agarwal, Jillian Banfield, Harry Beller, Nicholas Bouskill, Eoin Brodie, Rosemary Carroll, Baptiste Dafflon, Dipankar Dwivedi, Nicola Falco, Boris Faybishenko, Reed Maxwell, Peter Nico, Carl Steefel, Heidi Steltzer, Tetsu Tokunaga, Phuong A. Tran, Haruko Wainwright and Charuleka Varadharajan (2018) The East River, Colorado, Watershed: A mountainous community testbed for improving predictive understanding of multiscale hydrological–biogeochemical dynamics. *Vadose Zone Journal* **17** (1): 1-25.
- Deng, H., S Molins, D Trebotich, C Steefel, D DePaolo (2018) Pore-scale numerical investigation of the impacts of surface roughness: Upscaling of reaction rates in rough fractures, *Geochimica et Cosmochimica Acta* **239**: 374-389.
- Dwivedi, D., Carl I Steefel, Bhavna Arora, Michelle Newcomer, J David Moulton, Baptiste Dafflon, Boris Faybishenko, Patricia Fox, Peter Nico, Nic Spycher, Rosemary Carroll, Ken Williams (2018) Geochemical exports to river from the intra-meander hyporheic zone under transient hydrologic conditions: East River mountainous watershed, Colorado. *Water Resources Research* **54**: 8456-8477. DOI: [10.1029/2018WR023377](https://doi.org/10.1029/2018WR023377).
- Siriila-Woodburn, E.R., C.I. Steefel, K.H. Williams, J.T. Birkholzer (2018) Predicting the impact of land management decisions on overland flow generation: Implications for cesium migration in forested Fukushima watersheds. *Advances in Water Resources* **113**: 42-54.
- Deng, H., C.I. Steefel, S. Molins, D. DePaolo (2018) Fracture evolution in multi-mineral systems: The role of mineral composition, flow rate and fracture aperture heterogeneity. *ACS Earth Space Chem.* **2**: 112-124. DOI: [10.1021/acsearthspacechem.7b00130](https://doi.org/10.1021/acsearthspacechem.7b00130)
- Dwivedi, D., B. Arora, C.I. Steefel, B. Dafflon, R. Versteeg (2017) Hot spots and hot moments of nitrogen in a riparian corridor. *Water Resources Research* **54**: 205-222. DOI: [10.1002/2017WR022346](https://doi.org/10.1002/2017WR022346)
- Perdrial, N., A. Vazquez-Ortega, G. Wang, M. Kanematsu, K.T. Mueller, W. Um, C.I. Steefel, P. O'Day, J. Chorover (2018) Uranium speciation in acid waste-weathered sediments: The role of aging and phosphate amendments. *Applied Geochemistry* **89**: 109-120.

- Cao, B., A.G. Stack, C.I. Steefel, D.J. DePaolo, L.N. Lammers, Y. Hu (2017) Investigating calcite growth rates using a quartz crystal microbalance with dissipation (QCM-D). *Geochimica et Cosmochimica Acta* **222**: 269-283.
- Deng, H., M. Voltolini, S. Molins, C. Steefel, D. DePaolo, J. Ajo-Franklin, and L. Yang, (2017) Alteration and erosion of rock matrix bordering a carbonate-rich shale fracture. *Environmental Science and Technology* **51**: 8861-8868, DOI: 10.1021/acs.est.7b02063
- Li, Q., C.I. Steefel, Y-S Jun (2017) Deciphering calcium carbonate precipitation associated with CO₂ attack on cement using reactive transport modeling. *Environmental Science and Technology* **51**: 10861-10871, DOI: 10.1021/acs.est.7b00594.
- Arora, B., D. Dwivedi, N. Spycher, C. Steefel (2017) On modeling CO₂ dynamics in a flood Plain aquifer. *Procedia Earth and Planetary Science* **17**: 408-411
- Dwivedi, D, C Steefel, B Arora, G Bisht (2017) Impact of intra-meander hyporheic flow on nitrogen cycling. *Procedia Earth and Planetary Science* **17**: 404-407.
- Guo, J. B. Cao, C.I. Steefel, J. Chen, Y. Hu. (2017) Effects of sulfate and magnesium on cement degradation under geologic CO₂ sequestration conditions. *International Journal of Greenhouse Gas Control* **63**: 118-125.
- Molins, S., Trebotich, D., Miller, G. H. and Steefel, C. I. (2017) Mineralogical and transport controls on the evolution of porous media texture using direct numerical simulation. *Water Resources Research* **53**: 3645-3661. DOI:10.1002/2016WR020323
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