

Sergi Molins

Staff Scientist

Energy Geosciences Division | Lawrence Berkeley National Laboratory

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Profile

Reactive transport modeling from the pore to the watershed scale to address problems related to water, energy and the environment.

Expertise in the investigation of solute transport controls on interfacial reaction rates.

Model development and implementation (Fortran, C/C++, Python) in high performance codes for supercomputing environments.

Education

Ph.D., University of British Columbia, Vancouver, Canada	2007
Civil Engineer, Technical University of Catalonia, Barcelona, Spain	2001

Professional Experience

Staff Scientist, Lawrence Berkeley National Laboratory	2020–
Research Scientist, Lawrence Berkeley National Laboratory	2013–2020
Postdoctoral Fellow, Lawrence Berkeley National Laboratory	2008–2013
Teaching & Research Assistant, University of British Columbia	2002–2007
Research Assistant, Technical Univ. Catalonia & Earth Sci. Inst. Jaume Almera	2001–2002

Peer-reviewed Publications (Web of Science h-index: 20, Google Scholar h-index: 24)

1. Deng, H., Tournassat, C., Molins, S., Claret, F., & Steefel, C. I. (2021). A Pore-Scale Investigation of Mineral Precipitation Driven Diffusivity Change at the Column-Scale. *Water Resour. Res.*, 57(5), e2020WR028483. doi:10.1029/2020WR028483
2. Özgen-Xian, I., Navas-Montilla, A., Dwivedi, D., & Molins, S. (2021). Hyperbolic Reformulation Approach to Enable Efficient Simulation of Groundwater Flow and Reactive Transport. *Environ. Engin. Sci.*, 38(3), 181–191. doi:10.1089/ees.2020.0363
3. Molins, S., Soulaire, C., Prasianakis, N. I., Abbasi, A., Poncet, P., Ladd, A. J. C., et al. (2020). Simulation of mineral dissolution at the pore scale with evolving fluid-solid interfaces: review of approaches and benchmark problem set. *Comput. Geosci.* doi:10.1007/s10596-019-09903-x
4. Özgen-Xian, I., Kesserwani, G., Cavedes-Voullième, D., Molins, S., Xu, Z., Dwivedi, D., et al. (2019). Wavelet-based local mesh refinement for rainfall–runoff simulations. *J. Hydroinform.* doi:10.2166/hydro.2020.198
5. Molins, S., P. Knabner (2019) Multiscale approaches in reactive transport modeling, *Rev. Mineral. Geochem.* 85.
6. Molins, S., D. Trebotich, B. Arora, C.I. Steefel, H. Deng (2019). Multi-scale Model of Reactive Transport in Fractured Media: Diffusion Limitations on Rates. *Transport Porous Med.* doi:10.1007/s11242-019-01266-2

7. Deng, H., Molins, S., Trebotich, D., Steefel, C., & DePaolo, D. (2018). Pore-scale numerical investigation of the impacts of surface roughness: Upscaling of reaction rates in rough fractures. *Geochem. Cosmoch. Acta*, 239, 374–389. doi:10.1016/j.gca.2018.08.005
8. Deng, H., Steefel, C., Molins, S., & DePaolo, D. (2017). Fracture Evolution in Multimineral Systems: The Role of Mineral Composition, Flow Rate, and Fracture Aperture Heterogeneity. *ACS Earth and Space Chemistry*. doi:10.1021/acsearthspacechem.7b00130
9. Molins, S., D. Trebotich, G. Miller, C.I. Steefel (2017) Mineralogical and transport controls on the evolution of porous media texture using direct numerical simulation. *Water Resour. Res.*, doi:10.1002/2016WR020323
10. Deng, H., Fitts, J. P., Crandall, D., McIntyre, D., & Peters, C. A. (2015). Alterations of Fractures in Carbonate Rocks by CO₂-Acidified Brines. *Environ. Sci. Technol.*, 49(16), 10226–10234. doi:10.1021/acs.est.5b01980
11. Varadharajan, C., H. Beller, M. Bill, E. Brodie, M. Conrad, R. Han, C. Irwin, J. Larsen, H. Lim, S. Molins, C. Steefel, et al. (2017), Re-oxidation of Chromium(III) products formed under different biogeochemical regimes, *Environ. Sci. Technol.*, 10.1021/acs.est.6b06044.
12. Ajo-Franklin, J., M. Voltolini, S. Molins, and L. Yang (2018), Coupled processes in a fractured reactive system: a dolomite dissolution study with relevance to GCS caprock integrity, *In Geological Carbon Storage* (eds S. Vialle, J. Ajo-Franklin and J.W. Carey). doi:10.1002/9781119118657.ch9.
13. Ding, X., B. Kennedy, S. Molins, T. Kneafsey, and W. Evans (2017), Experimental studies and model analysis of noble gas fractionation in low-permeability porous media, *Geochem. Cosmoch. A.*, doi:10.1016/j.gca.2017.02.005.
14. Deng, H., S. Molins, C. Steefel, D. DePaolo, M. Voltolini, L. Yang, and J. Ajo-Franklin (2016), A 2.5D Reactive Transport Model for Fracture Alteration Simulation, *Environ. Sci. Technol.*, doi:10.1021/acs.est.6b02184.
15. Dwivedi, D., Arora, B., Molins, S., & Steefel, C. I. (2016). Benchmarking Reactive Transport Codes for Subsurface Environmental Problems. *In Groundwater Assessment, Modeling, and Management* (Vols. 1–0, pp. 299–316). CRC Press. doi:10.1201/9781315369044-20
16. De Baere, B., S. Molins, K. U. Mayer, and R. François (2016), Determination of mineral dissolution regimes using flow-through time-resolved analysis (FT-TRA) and numerical simulation, *Chem. Geol.*, 430, 1–12, doi:10.1016/j.chemgeo.2016.03.014.
17. Arora, B., N. Spycher, C.I. Steefel, S. Molins, M. Bill, M.E. Conrad, W. Dong, et al. (2016), Influence of hydrological, biogeochemical and temperature transients on subsurface carbon fluxes in a flood plain environment, *Biogeochem.*, 1–30, doi:10.1007/s10533-016-0186-8.
18. Cheng, Y., C. Hubbard, L. Li, N. Bouskill, S. Molins, L. Zheng, E. Sonnenthal, et al (2016), A Reactive Transport Model of Sulfur Cycling as Impacted by Perchlorate and Nitrate Treatments, *Environ. Sci. Technol.*, doi:10.1021/acs.est.6b00081.
19. Molins, S., J. Greskowiak, C. Wanner, and K.U. Mayer (2015), A benchmark for microbially mediated chromium reduction under denitrifying conditions in a biostimulation column experiment, *Comput. Geosci.*, 1–18, doi:10.1007/s10596-014-9432-0.
20. Beisman, J., R. Maxwell, A. Navarre-Sitchler, C.I. Steefel, and S. Molins (2015), ParCrunchFlow: an efficient, parallel reactive transport simulation tool for physically and chemically heterogeneous saturated subsurface environments, *Comput. Geosci.*, 1–20, doi:10.1007/s10596-015-9475-x.
21. Molins, S. (2015), Reactive interfaces in direct numerical simulation of pore-scale processes, *Rev. Mineral. Geochem.*, 80(1), 461–481, doi:10.2138/rmg.2015.80.14.
22. Steefel, C.I., C. Appelo, B. Arora, D. Jacques, T. Kalbacher, O. Kolditz, V. Lagneau, P. Lichtner, K.U. Mayer, J. Meeussen, S. Molins, D. Moulton, et al. (2015), Reactive transport codes for subsurface environmental simulation. *Comput. Geosci.*, 1–34.
23. Beller, H. R., L. Yang, C. Varadharajan, R. Han, H.C. Lim, U. Karaoz, S. Molins, M.A. Marcus, E.L. Brodie, C.I. Steefel, and P.S. Nico (2014), Divergent aquifer biogeochemical systems converge on similar and unexpected Cr(VI) reduction products, *Environ. Sci. Technol.*, 48(18), 10699–10706, doi:10.1021/es5016982.

24. Trebotich, D., M.F. Adams, S. Molins, C.I. Steefel, and C. Shen (2014), High-resolution simulation of pore-scale reactive transport processes associated with carbon sequestration, *Comput. Sci. Eng.*, 16(6), 22–31, doi:10.1109/MCSE.2014.77.
25. Molins, S., D. Trebotich, L. Yang, J.B. Ajo-Franklin, T.J. Ligocki, C. Shen, and C.I. Steefel (2014), Pore-scale controls on calcite dissolution rates from flow-through laboratory and numerical experiments, *Environ. Sci. Technol.*, 48(13), 7453–7460, doi:10.1021/es5013438.
26. Steefel, C.I., S. Molins, and D. Trebotich (2013), Pore scale processes associated with subsurface CO₂ injection and sequestration, *Rev. Mineral. Geochem.*, 77(1), 259–303, doi:10.2138/rmg.2013.77.8.
27. Molins, S., D. Trebotich, C.I. Steefel, and C. Shen (2012), An investigation of the effect of pore scale flow on average geochemical reaction rates using direct numerical simulation, *Water Resour. Res.*, 48(3), doi:10.1029/2011WR011404.
28. Druhan, J.L., C.I. Steefel, S. Molins, K.H. Williams, M.E. Conrad, and D.J. DePaolo (2012), Timing the onset of sulfate reduction over multiple subsurface acetate amendments by measurement and modeling of sulfur isotope fractionation, *Environ. Sci. Technol.*, 46(16), 8895–8902, doi:10.1021/es302016p.
29. Molins, S., K.U. Mayer, R.T. Amos, and B.A. Bekins (2010), Vadose zone attenuation of organic compounds at a crude oil spill site— Interactions between biogeochemical reactions & multicomponent gas transport, *J. Contam. Hydrol.*, 112(1-4), 15–29, doi:10.1016/j.jconhyd.2009.09.002.
30. Molins, S., K.U. Mayer, C. Scheutz, and P. Kjeldsen (2008), Transport and reaction processes affecting the attenuation of landfill gas in cover soils, *J. Environ. Qual.*, 37(2), 459, doi:10.2134/jeq2007.0250
31. Molins, S., and K.U. Mayer (2007), Coupling between geochemical reactions and multicomponent gas and solute transport in unsaturated media: A reactive transport modeling study, *Water Resour. Res.*, 43(5), doi:10.1029/2006WR005206.
32. Molins, S., J. Carrera, C. Ayora, and M.W. Saaltink (2004), A formulation for decoupling components in reactive transport problems, *Water Resour. Res.*, 40(10), doi:10.1029/2003WR002970.

Book Chapters, Reports, Manuals

- Spycher, N., Zhang, G., Sonnenthal, E., & Molins, S. (2021). TOUGHREACT-Brine: Supplement to TOUGHREACT-V4.0-OMP User's Guide for Modeling Concentrated Solutions and Osmosis Using the Pitzer Ion-Interaction Model. Retrieved from <https://escholarship.org/uc/item/2fz44294>
- Dwivedi, D., B. Arora, S. Molins, and C. I. Steefel (2016), Benchmarking reactive transport codes for subsurface environmental problems, in *Groundwater Assessment, Modeling, and Management*, pp. 299–316, CRC Press.
- Steefel, C.I., and S. Molins (2016), CrunchFlow: Software for modeling multicomponent reactive flow and transport. User's manual.
- Rutqvist, J., L. Blanco Martín, M. Hu, S. Molins, D. Trebotich, and J. Birkholzer (2016), Modeling coupled THM processes and brine migration in salt at high temperatures. Report number: LBNL-1006308.
- Rutqvist, J., L. Blanco-Martin, S. Molins, D. Trebotich, and J. Birkholzer (2015), Modeling coupled THM processes and brine migration in salt at high temperatures, Lawrence Berkeley National Laboratory (LBNL), Report number LBNL-191216.
- Mayer, K., R.T. Amos, S. Molins, and F. Gerard (2012), Reactive transport modeling in variably saturated media with MIN3P: Basic model formulation and model enhancements in Groundwater reactive transport models, pp 187–212. Bentham Science Publishers Ltd.

Invited Presentations

- Molins S, Trebotich D, Deng H & Steefel C, Hybrid Multiscale Model for Evolving Porous Media (Keynote), Goldschmidt 2019, August 18-23, 2019, Barcelona.
- Molins, S., D. Trebotich, C. Steefel (2017) Perspectives on reactive transport modeling at the pore scale, (Invited) Reactive Transport for the Earth and Environmental Sciences in the 21st Century Workshop, Amboise, France, October 3, 2017.
- Molins, S., D. Trebotich, C. Steefel (2017) Pore-scale controls on mineral dissolution and porous media evolution, (Invited) EOAS Colloquium, University of British Columbia, Vancouver, Canada, Nov 9, 2017.
- Molins, S., D. Trebotich, G. Miller, C.I. Steefel, M. Voltolini, J.B. Ajo-Franklin, B. DeBaere (2016), Representation of reactive interfaces in direct numerical simulation of pore-scale processes (*Invited*), Interpore Conference, May 9-12, 2016, Cincinnati, OH.
- Trebotich, D., S. Molins (*presenter*), C.I. Steefel, H. Deng (2016), Adaptive multiscale modeling of geochemical impacts on fracture evolution (*Invited*), AGU Fall Mtg., Dec 12-16, San Francisco CA.
- Molins, S., M. Day, J. Johnson, and C.I. Steefel (2015), Code interoperability in reactive transport modeling: the adaptive mesh refinement example (*Invited*), Goldschmidt Conference, Aug 16-21, Prague, Czech Republic.
- Molins, S. (2014), Bridging the gap from pore to continuum scales in reactive transport (*Invited*), Gordon Research Conference, Jul 6-11, Bates College, Lewiston, ME.
- Molins, S. (2013), Pore-scale simulation of reactive transport from experimentally-derived image data at high resolution (*Invited*), Berkeley Energy and Climate Lectures, Feb 19, UC Berkeley, CA.
- Molins, S., D. Silin, D. Trebotich, and C.I. Steefel (2011), Direct pore scale numerical simulation of precipitation and dissolution (*Invited*), Goldschmidt Conf., Aug 14-19, Prague, Czech Republic.

Software Disclosures and Contributions

- Amanzi-ATS: A flexible and extensible parallel flow and reactive transport simulation capability for environmental applications and a code for solving ecosystem-based, integrated, distributed hydrology. Single three-clause BSD license, with copyright asserted by each LANL, LBNL, ORNL, PNNL on the contributions of its employees. Public repository: github.com/amanzi.
- MIN3P/MIN3P-Dusty: A numerical model to simulate multicomponent reactive mass transport and the Dusty Gas Model (DGM). K.U. Mayer, S. Molins, and J. VanderKwaak. Intellectual property disclosure as *University Research Product*, Univ. British Columbia File No. 14-143, Oct 2015.
- CrunchFlow: Software for modeling multicomponent reactive flow and transport. C.I. Steefel, S. Molins. Software disclosure LBNL File No 2016-015, Nov 2015. BSD open-source license, copyright held by UC Regents through LBNL. Public repository: bitbucket.org/crunchflow/crunchtope-dev.
- Alquimia: A unified API and wrapper library for existing geochemical codes. B. Andre. Software disclosure LBNL Ref. 2013-119. BSD open-source license, copyright held by UC Regents through LBNL. Public repository: github.com/LBL-EESA/alquimia-dev.
- Chombo-Crunch: An adaptive mesh refinement embedded-boundary simulator for pore scale reactive transport and hybrid multiscale modeling. Unlicensed. <https://paperpile.com/shared/OHZwrr>

Professional Development, Activities and Service

- Memberships · American Geophysical Union, Geochemical Society, Interpore Society, American Chemical Society
- Assoc. Editor:· Water Resources Research (2017-present)
- Peer reviewer · (Journals) *ACS ES&T Water*, *ACS Space and Earth Chemistry*, *Appl. Geochem.*, *Acc. Chem. Res.*, *Int. J. Greenh. Gas Control*, *J. Petrol. Sci. Engin.*, *Water Resour. Res.*,

- Environ. Sci. Technol., Am. J. Sci., Waste Manage., J. Hydrol., Hydrol. Earth System Sci., J. Contamin. Hydrol., J. Environ. Qual., Adv. Water Resour., Geochim. Cosmochim. A., Comp. Geosci., Int. J. Heat Mass Transf., Geophys. Res. Lett., Transp. Porous Med., Environ. Engin. Sci., J. Geophys. Res.: Biogeosci.*
- (Proposals) *SFA Review, Biological and Environmental Research Program, DOE Office of Science, Netherlands Organisation for Scientific Research (NWO), Agence Nationale de la Recherche, France; Hans-Fischer Fellowship, Tech Univ Munich*
- Convener
- *Reactive Transport Modeling: A Cutting-Edge Tool for Investigating Coupled Processes, ACS Spring Meeting, Virtual, April 9, 2021*
 - *Reactive Transport in Real Rocks: From the Pore to the Field Scale (H088) AGU Fall Meeting, Virtual, Thursday, 10 December 2020*
 - *Evolving porous media and coupled chemical and physical processes, Interpore conference, New Orleans, Louisiana, May 16, 2018*
 - *Modeling of Subsurface Biogeochemical Processes at the XVIII Conference on Computational Methods in Water Resources (CMWR 2010), Barcelona, Jun 21-24, 2010.*
 - *Benchmarking Next-Generation Reactive Transport Models for Predicting Watershed Biogeochemical Cycling at the 2015 AGU Fall Meeting, San Francisco, Dec 14-18, 2015.*
- Workshops
- (Participant) *Environmental System Science workshop on Model-Data Integration, U.S. DOE, Office of Science, Potomac, MD, April 30 – May 1, 2015.*
 - (Participant) *Environmental System Science Working Groups 2017 Annual Meeting, U.S. DOE, Office of Science, Potomac, MD, April 24, 2017.*
- Training
- *Python Bootcamp at Berkeley, Brower Center, UC Berkeley, Aug 26-28, 2013.*
 - *Web Programming for Scientists, Software Carpentry, LBNL, Mar 13, 2015.*
 - *Intro to Relational and Non-Relational Databases for Researchers, Software Carpentry, LBNL, Apr 7, 2016.*
 - *Managing Research Software Projects, Software Carpentry, LBNL, Jan 18, 2017.*
 - *Gender Bias in Academic Publishing, Elsevier Publishing Campus, webinar, May 11, 2017.*
 - *Argonne Training Program on Extreme-Scale Comp, St. Charles IL, Jul 30-Aug 11, 2017*
 - *Wiley Editor Seminar: Diversity in Your Journal Community, Virtual May 11, 2021*
- Supervisor
- (LBNL) Zexuan Xu, Ilhan Ozgen-Xian, Bhavna Arora (former), Baky Kallemov (former)
- Committees
- (Hiring, UC Berkeley) Microbial Modeling Postdoctoral Researcher, 2021
 - (Hiring, LBNL) Research Scientist in Integrated Hydrological Modeling, 2019
 - (Hiring, LBNL) Research Scientist in Watershed Reactive Transport Modeling, 2016.
 - (PhD thesis examiner) Gamazo, P., *A code for multiphase reactive transport modeling of concentrated solutions under extreme dry conditions*, Tech. Univ. Catalonia, Dec 2010.

Awards and Scholarships

R&D100 Award for Amanzi-ATS	2021
R&D100 Award for CrunchFlow	2017
Winner, US DOE <i>Life at the Frontiers of Energy Research</i> Video Contest for <i>Carbon in Underland</i> (youtu.be/gr9cznZFuIc)	2011
SPOT Recognition Award, LBNL	2011
Egil H. Lorntzen Scholarship, UBC	2006
University Graduate Fellowship, UBC	2003-2005
Thomas and Marguerite MacKay Memorial Scholarship, UBC	2003