

## SERGI MOLINS

Research Scientist

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## Research Profile

Reactive transport modeling from the pore to the watershed scale.

Elucidation of processes affecting the formation of effective reaction rates at different spatial scales in subsurface applications relevant to energy and the environment.

Model development and implementation in computer codes, specializing in interfaces between geochemical codes and HPC simulators of flow and transport.

Current projects: Center for Nanoscale Control of Geologic CO<sub>2</sub> (NCGC), Genomes to Watersheds Scientific Focus Area (SFA 2.0), Interoperable Design of Extreme-scale Application Software (IDEAS), Advanced Simulation Capability for Environmental Management (ASCEM), Used Fuel Disposition (Salt Migration), Multi-Scale Modeling of Geochemical Impacts on Fracture Evolution (LDRD).

## Education

Ph.D., University of British Columbia, Vancouver 2007

Civil Engineer, Technical University of Catalonia, Barcelona 2001

## Professional Experience

Research Scientist, Lawrence Berkeley National Laboratory 2013–

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

## Publications

Molins, S. (2015). Reactive Interfaces in Direct Numerical Simulation of Pore-Scale Processes. *Rev. Mineral. Geochem.*, 80(1):461–481

Beisman, J., Maxwell, R., Navarre-Sitchler, A., Steefel, C., and Molins, S. (2015). ParCrunchFlow: an efficient, parallel reactive transport simulation tool for physically and chemically heterogeneous saturated subsurface environments. *Comput. Geosci.*, pages 1–20

Molins, S., Trebotich, D., Yang, L., Ajo-Franklin, J. B., Ligocki, T. J., Shen, C., and Steefel, C. I. (2014b). Pore-scale controls on calcite dissolution rates from flow-through laboratory and numerical experiments. *Environ. Sci. Technol.*, 48(13):7453–7460

- Molins, S., Greskowiak, J., Wanner, C., and Mayer, K. (2014a). A benchmark for microbially mediated chromium reduction under denitrifying conditions in a biostimulation column experiment. *Comput. Geosci.*, pages 1–18
- Steeffel, C., Appelo, C., Arora, B., Jacques, D., Kalbacher, T., Kolditz, O., Lagneau, V., Lichtner, P., Mayer, K., Meeussen, J., Molins, S., Moulton, D., Shao, H., Simunek, J., Spycher, N., Yabusaki, S., and Yeh, G. (2014). Reactive transport codes for subsurface environmental simulation. *Comput. Geosci.*, pages 1–34
- Beller, H. R., Yang, L., Varadharajan, C., Han, R., Lim, H. C., Karaoz, U., Molins, S., Marcus, M. A., Brodie, E. L., Steefel, C. I., and Nico, P. S. (2014). Divergent aquifer biogeochemical systems converge on similar and unexpected Cr(VI) reduction products. *Environ. Sci. Technol.*, 48(18):10699–10706
- Trebotich, D., Adams, M. F., Molins, S., Steefel, C. I., and Shen, C. (2014). High-resolution simulation of pore-scale reactive transport processes associated with carbon sequestration. *Comput. Sci. Engin.*, 16(6):22–31
- Steeffel, C. I., Molins, S., and Trebotich, D. (2013). Pore scale processes associated with subsurface CO<sub>2</sub> injection and sequestration. *Rev. Mineral. Geochem.*, 77:259–303
- Druhan, J. L., Steefel, C. I., Molins, S., Williams, K. H., Conrad, M. E., and DePaolo, D. J. (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
- Molins, S., Trebotich, D., Steefel, C. I., and Shen, C. (2012). An investigation of the effect of pore scale flow on average geochemical reaction rates using direct numerical simulation. *Water Resour. Res.*, 48(3)
- Molins, S., Mayer, K. U., Amos, R. T., and Bekins, B. A. (2010). Vadose zone attenuation of organic compounds at a crude oil spill site - Interactions between biogeochemical reactions and multicomponent gas transport. *J. Contam. Hydrol.*, 112(1-4, SI):15–29
- Molins, S., Mayer, K. U., Scheutz, C., and Kjeldsen, P. (2008). Transport and reaction processes affecting the attenuation of landfill gas in cover soils. *J. Environ. Qual.*, 37(2):459–468
- Molins, S. and Mayer, K. U. (2007). Coupling between geochemical reactions and multicomponent gas and solute transport in unsaturated media: A reactive transport modeling study. *Water Resour. Res.*, 43(5)
- Molins, S., Carrera, J., Ayora, C., and Saaltink, M. (2004). A formulation for decoupling components in reactive transport problems. *Water Resour. Res.*, 40(10)

## Book Chapters

- Mayer, K., Amos, R. T., Molins, S., and Grard, F. (2012). *Groundwater reactive transport models*, chapter Reactive transport modeling in variably saturated media with MIN3P: Basic model formulation and model enhancements, pages 187–212. Bentham Science Publishers Ltd

## Selected Invited Presentations

- Molins, S., Day, M., Johnson, J., and Steefel, C. I. (2015). Code Interoperability in Reactive

- Transport Modeling: The Adaptive Mesh Refinement Example. In *Goldschmidt Conference*, Prague, Czech Republic
- Molins, S. (2014). Bridging the Gap from Pore to Continuum Scales in Reactive Transport. In *Gordon Research Conference*, Bates College, Lewiston, ME
- Molins, S. (2013). Pore-scale simulation of reactive transport from experimentally-derived image data at high resolution. In *Berkeley Energy and Climate Lectures*, Univ. California, Berkeley
- Molins, S., Silin, D., Trebotich, D., and Steefel, C. I. (2011). Direct pore scale numerical simulation of precipitation and dissolution. In *Goldschmidt Conference*, Prague, Czech Republic

## Professional Activities

- Memberships      Geochemical Society, American Geophysical Union
- Reviewing          *Int. J. Greenh. Gas Control, J. Geophys. Res. Solid Earth, 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. Acta, Comp. Geosci., Int. J. Heat Mass Transf., and Geophys. Res. Lett.*
- Organization of conference sessions      *Modeling of Subsurface Biogeochemical Processes at the XVIII Conference on Computational Methods in Water Resources (CMWR 2010)*, Barcelona, June 21-24, 2010.
- Academic Committees      Examiner of PhD thesis *A code for multiphase reactive transport modeling of concentrated solutions under extreme dry conditions* by P.A. Gamazo, Technical Univ. Catalonia, Barcelona, Dec. 20, 2010.

## Awards and Scholarships

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| Winner, US DOE Life at the Frontiers of Energy Research Video Contest, for the video <i>Carbon in Underland</i> ( <a href="http://youtu.be/gr9cznZFuIc">youtu.be/gr9cznZFuIc</a> ) | 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      |