

[Form 2 (to be reported to Committee on Countermeasures for Contaminated Water Treatment and to be disclosed to public)]

Technology Information	
Area	5, 6 (Select the number from "Areas of Technologies Requested")
Title	Reactive transport modeling for understanding the long-term fate of radionuclides in groundwater and for evaluating remediation strategies
Submitted by	Lawrence Berkeley National Laboratory: Carl Steefel, Nic Spycher, James Davis, Haruko Murakami-Wainwright, Jens Birkholzer
<p>1. Overview of Technologies (features, specification, functions, owners, etc.)</p> <p>Reactive transport modeling is a critical component for understanding the long-term fate of radionuclides in groundwater and soils, as well as for evaluating the effectiveness of remediation strategies and site cleanup alternatives. Although the current focus at the Fukushima Daiichi NPP site is primarily on understanding and managing groundwater flow through the site and into the ocean, geochemical reactions could potentially have a significant impact on the long-term fate of radionuclides such as cesium, tritium, and strontium, and thus need to be understood if predictive models or successful remediation strategies are to be developed. Even if hydraulic and decontamination countermeasures are successful in reducing most of the local groundwater contamination, radionuclides may remain in the silt and clay fractions of impacted soil. Changes in ionic strength and/or in the concentration of specific constituents that compete for sorption sites – a possible result of hydraulic measures moving the local seawater-freshwater boundaries – could strongly influence the sorption-desorption and other reactive behaviors of radionuclides, potentially leading to contaminant remobilization after remediation.</p> <p>In fact, high concentrations of cesium have been discovered in groundwater at the Fukushima Daiichi NPP site, even though it had originally been assumed that cesium would be immobile as a result of strong sorption. Similar observations have been made at the Hanford 200 Area, where cesium migrated to significant depths because of the high ionic strength of the solutions moving through the vadose zone (Zachara et al, 2002; Steefel et al, 2003; Steefel et al, 2005). These findings suggest that ignoring geochemical reactions could potentially cause a costly failure of any proposed remedial alternative. For example, reducing the up-gradient groundwater flow could draw more seawater into the site, potentially promoting the desorption of cesium and increasing its flux into the ocean. Such geochemistry-governed radionuclide transport, which has been reported at many other sites [e.g., Bea et al., 2013; Steefel et al., 2003; Davis et al, 2004], can be assessed with advanced reactive transport models that take into account the subsurface physical and geochemical heterogeneities and represent complex groundwater flow and salinity conditions.</p> <p>There are advanced reactive transport simulation codes developed under the US Department of Energy (DOE) such as the TOUGH family of codes (<a href="http://esd.lbl.gov/research/projects/tough/">esd.lbl.gov/research/projects/tough/</a>), CrunchFlow (<a href="http://www.csteefel.com/CrunchFlowIntroduction.html">www.csteefel.com/CrunchFlowIntroduction.html</a>), and also the multi-lab code development ASCEM (<a href="http://esd.lbl.gov/research/projects/ascem/">esd.lbl.gov/research/projects/ascem/</a>) that can address these issues. Key features of these simulators relevant to the Fukushima site include:</p> <ul style="list-style-type: none"> <li>- Complex geochemical reactions for describing the effect of variable groundwater geochemistry at the freshwater-seawater boundary [Steefel et al., 2003; Xu et al., 2008]</li> <li>- Groundwater flow with variable density for simulating seawater intrusion</li> <li>- High-performance computing resources for enabling high resolution large-scale simulations</li> <li>- Global sensitivity and uncertainty analysis capabilities for addressing the uncertainty in various parameters [Finsterle, 1999; Freshley et al., 2012]</li> <li>- Optimization capabilities of remediation and counter-measure strategies [Finsterle, 2006]</li> </ul> <p>In addition, LBNL has extensive knowledge and experiences in characterizing geochemical reactions at contaminated sites and developing conceptual and numerical reactive transport models [Davis et al, 2004]. Such experience, along with the numerical and computational capabilities at Lawrence Berkeley National Laboratory, will certainly contribute to improvement in our understanding of radionuclide transport as well as the designs for effective remedial strategies at the Fukushima Daiichi NPP site.</p>	

2. Notes (Please provide following information if possible.)

- Technology readiness level (including cases of application, not limited to nuclear industry, time line for application)

The reactive transport simulators mentioned above are ready to use.

- Challenges

To develop the conceptual and numerical models of groundwater flow and geochemistry, various types of data are needed. These include water table elevations, subsurface permeability, evapotranspiration rates, soil and subsurface ion exchange properties, and mineralogy.

- Others (referential information on patent if any). NO RELATED PATENTS

Bea, B. A., H.M. Wainwright, N. Spycher, B. Faybishenko, S. S. Hubbard, M. Denham, Identifying key controls on acidic-U(VI) plume behavior at the Savannah River Site, using reactive transport modeling, *Journal of Contaminant Hydrology*, 151, 34-54, ISSN 0169-7722, 2013.

Davis, J.A., S.B. Yabusaki, C.I. Steefel, J.M. Zachara, G.P. Curtis, G.D. Redden, L.J. Criscenti, B.D. Honeyman, Assessing conceptual models for subsurface reactive transport of inorganic contaminants. *EOS* 84(44) (2004) 449, 455.

Finsterle, S., iTOUGH2 user's guide, LBNL-40040, 1999.

Finsterle, S., Demonstration of optimization techniques for groundwater plume remediation using iTOUGH2, *Environmental Modelling & Software* 21.5, 665-680, 2006.

Freshley, M., et al., Advanced Simulation Capability for Environmental Management (ASCEM) Phase II Demonstration", ASCEM-SITE-2012-01, 2012.

Steefel, C.I., Carroll, S., Zhao, P., and Roberts, S. (2003), Cesium migration in Hanford sediment: A multi-site cation exchange model based on laboratory transport experiments. *J. of Contaminant Hydrology* **67**, 219-246.

Steefel, C.I., D. DePaolo, and P.C. Lichtner, 2005, Reactive transport modeling: An essential tool and a new research approach for the Earth sciences, *Earth and Planetary Science Letters* **240**: 539-558.

Xu, T., et al. TOUGHREACT User's Guide: A Simulation Program for Non-isothermal Multiphase Reactive Geochemical Transport in Variably Saturated Geologic Media, V1. 2.1. No. LBNL-55460-2008. Ernest Orlando Lawrence Berkeley National Laboratory, Berkeley, CA (US), 2008.

Zachara, J.M., Smith, S.C., Liu, C., McKinley, J.P., Serne, R.J., Gassman, P.L., 2002. Sorption of Cs+ to micaceous subsurface sediments from the Hanford site, USA. *Geochimica et Cosmochimica Acta* 66, 193– 211.