Acronym	Topic description	Lead	Members
Poro-perm	This benchmark focuses on five hypothetical scenarios to evaluate formulations and compare implementations for permeability-porosity relationships in reactive transport models. Porosity changes are induced by mineral dissolution-precipitation reactions and the Carman-Kozeny relationship is used to describe changes in permeability as a function of porosity. Simulated reactive processes include: multicomponent aqueous complexation, kinetic surface-controlled reversible mineral dissolution and precipitation, coupling of dissolution-precipitation induced porosity change and fluid flow processes. One and two dimensional advective-diffusive transport simulations are conducted in saturated porous media.	Mingliang Xie	Francis Claret Aurelie Chagneau Dirk Mallants Olivier Bildstein Diederik Jacques Uli Mayer Carl Steefel
MCD	The benchmark problem is based on a multi-component advective-diffusive column experiment that was carried out with compacted bentonite (Mäder et al. 2012), at constant temperature, constant confining pressure, and constant hydraulic gradient. Deuterium was used as a tracer and there was a moderate contrast in composition between the infiltrating fluid and the initial pore water in the clay plug, including differences in chloride and sulfate. An increasing degree of complexity is developed comprising 5 steps: (1) a non-reactive single-porosity base case, (2) addition of reactive minerals (gypsum, calcite), (3) addition of ion-exchange capacity, (4) adding a micro-porosity subjected to charged surfaces with ion-exchange modelled as a DL process, and (5) adding a treatment of micro-porosity with one part of the fixed charge being treated as surface complexation (representing a Stern layer) and the remaining part being associated with a DL.	Peter Alt-Epping	Uli Mayer Carl Steefel S. Sevinc Sengor Mingliang Xie
Cr Isotopes	Simulated were processes that are relevant with respect to the Cr(VI) contamination: Groundwater Cr(VI) concentrations are controlled by the dissolution of sparingly soluble Cr(VI) bearing jarosite ($KFe_3(SO_4)_{1.8}(CrO_4)_{0.2}(OH)_6$), which is the dominant Cr(VI) bearing mineral phase within the saturated zone. Infiltrating rainwater and groundwater table variations leads to an additional dissolution of high loads of highly soluble chromatite ($CaCrO_4$) first of all present in the unsaturated zone. Once dissolved, Cr(VI) is reduced to Cr(III) by the presence of Fe^{2+} bearing minerals such as biotite, chlorite, hornblende, epidote and magnetite. Cr(III) then precipitates as $Cr(OH)_3$ or as a mixed Fe-Cr hydroxide. A current minimal Cr(VI) reduction efficiency of 32% along a 120 m long flow path was estimated by measuring Cr isotopes and applying a Rayleigh fractionation model (Wanner et al., 2012).	Christoph Wanner	Peter Alt-Epping Richard Amos Uli Mayer Steve B Yabusaki Carl Steefel
Multi-Rate	The here proposed benchmark problem consists of a 1D multi-component reactive transport model has been developed by Liu et al (2008) to explain the U(VI) desorption behavior in columns filled with U(VI) contaminated sediments from the Hanford 300A area. The model accounts for intra-grain diffusion-limited adsorption of U(VI) on multiple time scales via multi-rate surface complexation (SC) kinetics. In addition to the multi-rate SC kinetics at the microscopic scale, U(VI) leaching in the heterogeneous field textured sediments was also impacted by dual domain mass-transfer between immobile and mobile pore water at the macroscopic scale. The Benchmark problem set consists of 3 parts: (i) Principal problem: Multi-rate surface complexation and 1D transport in a single domain with constant	Janek Greskowiak	Uli Mayer Peter Alt-Epping Jin-Ping Gwo Jun Yin Diederik Jacques Carl Steefel

	hydrochemical composition at the column inlet. (ii) Component problem 1: Principal problem with inclusion of dual domain mass- transfer (Original model of Liu et al., 2008) (iii) Component problem 2: Component problem 1 with non-constant hydrochemical composition at the column inlet.		
Cement-Clay	In Europe, cementitious materials are considered to be used in many concepts of radioactive waste deep underground disposal. The challenge of this benchmark is linked to the complexity of the chemical reactions. Its mineralogy includes 10 primary phases, where the concrete contains 7 primary phases with crystalline form of C-S-H formation taken into account. Reaction kinetics has been considered for 10 phases, whereas other minerals have been processed at local equilibrium.	Francis Claret	Olivier Bildstein Benoit Cochepin Diederik Jacques Jean-Eric Lartigue Uli Mayer Hans Meeussen Isabelle Munier Ingmar Pointeau Danyang Su Sanheng Liu Nicolas Marty Eric Gaucher Carl Steefel
Fractured cement	This benchmark presents an application of a simplified 2D model of chemical degradation for a cracked concrete under near surface disposal conditions. The objective is to gain an improved understanding of the rate of degradation of the cracked concrete structure and finally its impact on transport of radionuclides and chemotoxic components. Chemical degradation of concrete affects physical and mechanical properties and consequently accelerates migration of radionuclides from the cementitious engineered barriers. This benchmark is performed in several steps, starting with dissolution of only one mineral (portlandite) and constant physical properties (porosity, bulk density…). The problem is then extended to evolving material properties and to more complex mineralogy. Final problem involves also leaching of complexing contaminant where also sorption properties change.	Diederik Jacques	Janez Perko Carl Steefel Hans Meeussen Laurent Dewindt Georg Kosakowski Uli Mayer
ARD	Dissolved inorganic and organic chemicals are commonly affected by a variety of physical and chemical processes, which influence their fate and mobility, but also alter the geochemical composition of soils and aquifer sediments. This is particularly true in the vadose zone, where the exchange of gases with the atmosphere can enhance the progress of biogeochemical reaction processes. This benchmark includes the solution of Richards equation for variably-saturated flow, and also the mass balance equations for advective-diffusive solute transport and diffusive gas transport. Biogeochemical reactions are described by a partial equilibrium approach, using equilibrium-based law-of-mass-action relationships for fast reactions, and a generalized kinetic framework for reactions that are relatively slow in comparison to the transport time scale.	Uli Mayer	Steve B Yabusaki Carl Steefel Diederik Jacques Olaf Kolditz Peter Alt-Epping
1D Uranium Bio	The benchmark addresses the coupled process modeling of hydrology and biogeochemical reactive transport. The principal benchmark problem involves the injection of lactate into a confined uranium contaminated aquifer via the four perimeter wells of a five-spot well pattern and simultaneous withdrawal from the central well. The lactate groundwater amendment stimulates indigenous microorganisms to catalyze the immobilization of residual post-ISR U(VI) to sparingly soluble U(IV) mineral. In the 1-D simulation, the uranium bioreduction rate will progressively increase because of the dependence on growing FeRB biomass.	Steve Yabusaki	S. Sevinc Sengor Luanjing Guo Sergi Molins Carl Steefel
Ureolityically Driven	Processes involved in this system are: 1-D flow in a saturated, homogeneous porous media driven by fixed hydraulic heads, aqueous rate limited hydrolysis of urea, kinetic precipitation	Luanjing Guo	S. Sevinc Sengor Peter Tsai Yilin Fang

			Carl Steefel
	and/or dissolution of calcium carbonate mineral, aqueous equilibrium reactions involving Ca2+, HCO3-, H+, and NH4+, solid-solution reactions (adsorption), and solution-media interactions (changes in media properties such as porosity and permeability). The objectives of numerical simulation are to study the nonlinear coupling effects among various processes and to predict the temporal and spatial distribution of mineral precipitates.		
Cr-Reduction	The focus of this benchmark problem is on the simulation of microbially mediated redox reactions with the explicit inclusion of the microbial community dynamics and their impacts on reaction rates. Simulated reactive processes include: multicomponent aqueous complexation; kinetically-controlled mineral precipitation and dissolution; biologically-mediated reactions, and biomass growth and decay. Rate expressions for microbially mediated redox reactions include kinetic limitations (Monod and inhibition terms) as well as thermodynamic limitations. Both catabolic (energy) and anabolic pathways (biomass growth) are considered in the microbially mediated reactions [Rittman and McCarty, 2001]. One-dimensional advective and diffusive transport are simulated using the global implicit approach to coupling transport and reactions. The microbial biomass is assumed to be exclusively non-planktonic and thus not subject to transport.	Sergi Molins	Janek Greskowiak Christoph Wanner Uli Mayer Carl Steefel
Concrete Carbonation	Atmospheric carbonation of concrete in unsaturated conditions is a complex process that involves intricate coupling between the concomitant drying (ventilation) and resaturation (from the site) of different cementitious components and the chemical degradation due to the diffusion of carbon dioxide. For this purpose, a series of simulations have been designed to explore the influence of the coupling between CO_2 gaseous/aqueous diffusion and the flow of water. These simulations are proposed as a benchmarking exercise consisting of different steps with progressive complexity, including case 1: the drying of concrete overpack; case 2: the carbonation process at constant water saturation; case 3: the fully coupled carbonation process.	Olivier Bildstein	Diederik Jacques Nikos Leterrier Benoît Bary Pascal Thouvenot Isabelle Munier Benoit Cochepin Uli Mayer Javier Samper Peter Alt-Epping Jérôme Corvisier Carl Steefel
Uranium reoxidation	The benchmark problem consists of the numerical simulation of batch experiments using the multicomponent biogeochemical reaction network (Part (a)); numerical simulation of the biogeochemical reaction network of Part (a) using a 2-D reactive transport model with constant hydrochemical composition and temporary slow injection of lactate in the middle of the domain (Part b)); Part (b) including surface complexation of U(VI) onto hematite surfaces (Part (c)). The aqueous speciation involving major ions, precipitation/dissolution of solid phases including UO_2, hematite, siderite, and mackinawite are considered as equilibrium reactions. Kinetic reactions are defined for sulfate bioreduction, Fe(III) bioreduction, U(VI) bioreduction, Fe(III) reduction by HS, U(VI) oxidation by Fe(III), and precipitation/dissolution of sulfur.	Sevinc Sengor	Diederik Jacques Janek Greskowiak Uli Mayer Sergi Molins Luanjing Guo Nicolas Spycher Carl Steefel
Maqarin	The Maqarin site in Jordan has been investigated for three decades as a natural analogue for the long term changes of	Haibing Shao	Haibing Shao Mingliang Xie

| | materials in contact with hyper-alkaline solutions. Similar processes are expected in radioactive waste disposal sites, where cement based materials are in contact with natural rocks or other e.g. clay based materials. Steefel and Lichtner (1998) has been using a simple geochemical model to investigate the local geochemical alterations and induced porosity changes for the Maqarin marl rock in contact with the hyper-alkaline solution. Inspired by that, the new setup includes several clay and zeolite minerals, considers cation exchange processes, and a solid solution model for cement phases. The model predicts that the pore space will clog after several hundred years at a distance of 5 – 10 mm from the contact to the hyper-alkaline solution. | | Carl Steefel |