EFFECTS OF ALTERNATE FLOW PATHWAYS ON WATER CHEMISTRIES IN REACTIVE TRANSPORT SIMULATIONS OF THE AMBIENT UNSATURATED ZONE AT YUCCA MOUNTAIN, NEVADA

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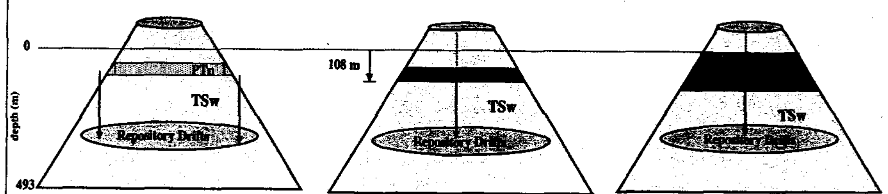
Abstract

The manner and extent to which groundwater compositions evolve along flow pathways are determined mainly by thermohydrologic conditions, the types of reactive materials encountered, and the interaction times with those materials. Simulated groundwater compositions vary significantly depending on whether or not the flow model includes lateral diversion of infiltrating waters, or preferential flow pathways in variably-saturated materials. To assist in the technical review of any license application for the proposed nuclear waste repository at Yucca Mountain (YM), NV, we developed a reactive transport model for the ambient hydrogeochemical system at Yucca Mountain. The model simulates two phase, non-isothermal, advective and diffusive flow and transport through one dimensional, matrix and fracture continua (dual permeability) containing ten kinetically reactive hydrostatigraphic layers in the vicinity of the SD-9 borehole at YM. In this presentation, we emphasize how uncertainties in ambient UZ flow pathways can lead to differences in simulated groundwater compositions. Furthermore, we note that data and characterization on the reactivity of rock units as fast, slow, or inert will help guide the improvement of reactive transport models in the unsaturated zone.

Alternative Flow Pathways



Case 1: Base case, no PTn unit

- Upper model boundary is Top of TSw
- Infiltrating water has revised analytical colluvium water composition
- Fracture-dominated flow through TSw
- Travel time through PTn: 0 years

Case 2: Base case, thin PTn unit

- Upper model boundary is Top of PTn
- Infiltrating water has revised analytical PTn pore water composition
- Matrix-dominated flow through 12 m thick section of PTn unit
- Fracture-dominated flow through TSw
- Travel time through PTn: 1,200 years

Case 3: Base case, thick PTn unit +/- lateral diversion

- Upper model boundary is Top of PTn
- Infiltrating water has revised analytical PTn pore water composition
- Matrix-dominated flow in arbitrarily thick (120 m) section of PTn unit; the additional thickness is a surrogate for lateral flow in the PTn
- Fracture-dominated flow through TSw
- Travel time through PTn: 12,000 years

Basic Model Properties (Cases 1-3)

Groundwater flow: Rock matrix and fracture networks in the unsaturated zone (UZ) are depicted as interacting porous continua. Heat/water flow between continua are controlled by:

- Darcy's law coupled with constitutive relationships and equations
- van Genuchten function with Mualem assumption for moisture retention/relative permeability
- the active fracture model (Liu et al., 1998)
- parameter values adopted from CRWMS M&O (2001).

Hydrostratigraphy: Nine (Case 1) or ten (Cases 2, 3) different hydrostratigraphic units bounded by the ptn26 and tsw38 layers (CRWMS, 2000). Each model unit is:

- horizontally-oriented with isotropic hydraulic properties
- defined by chemically and hydraulically distinct matrix and fracture continua
- occupied by different volumetric proportions of kinetically reactive phases.

Code: MULTIFLO version 1.5 (Painter et al., 2001).

Gridding: a 56 cell structured grid with a mixed upper boundary condition (i.e. specified gas pressure, temperature and liquid flux) and a gravity drainage lower boundary condition.

Geochemical Model: All 3 cases consider:

- dissolved species and gas: Cl^-, Ca^{2+}, H^+, HCO_3^-, $CO_2(aq)$, CO_3^{2-}, $SiO_2(aq)$, $HSiO_3^-$, $Al(OH)_4^-$, Na^+, K^+, OH^-, and Al^{3+}, and $CO_2(g)$
- kinetically reactive phases: low albite, calcite, rhyolitic glass, amorphous silica, and endmember Na, Ca, and K-smectites.

Results: Simulated Water Compositions

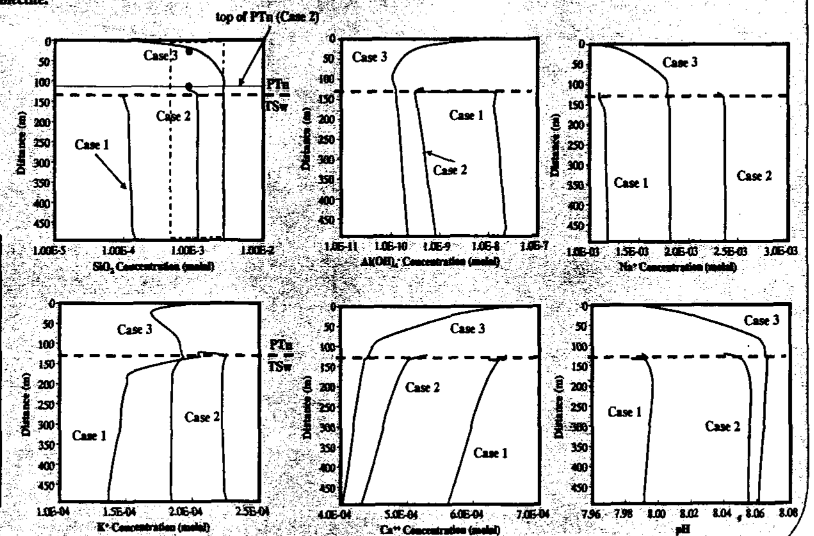
Differences in simulated matrix pore water compositions for Cases 1-3 under ambient quasi steady state conditions are shown below. The shaded region shows the range of revised analytical SiO_2 concentrations from YM (Browning et al., 2000; Browning and Murphy, 2002). Water compositions in glass-rich layers (i.e. PTn) are controlled by glass dissolution rates and the formation of smectite.

WATER COMPOSITIONS

The infiltrating and initial water compositions used to constrain boundary/initial conditions in our model are shown below.

Revised analytical matrix pore water compositions are from Browning et al., 2000.

Groundwater Component	Colluvium (Cases 1 and 3)	[1]PTn Pore water (Case 2)
pH	7.99	8.04
Ca (mg/L)	14.00	22.7
Na (mg/L)	25	53
$SiO_2(aq)$ (mg/L)	5.8	48.6
K (mg/L)	8	8
Al (mg/L)	1.3e-5	1.3e-5
HCO_3^- (mg/L)	114.1	115.3
CO_3^{2-} (mg/L)	0.72	0.64
Cl (mg/L)	10.0	6.0



Conclusions/Discussion

Even when extensive site characterization data are available, as is the case for YM, it may not be possible to uniquely constrain groundwater flow pathways through variably saturated, fractured, and heterogeneous rock layers. This presentation, for example, depicts three very different conceptualizations for UZ groundwater flow pathways at YM based on plausible interpretations of the same hydrogeostratigraphic data.

Our simulations illustrate that different conceptual models for groundwater flow can produce very dissimilar predictions of groundwater compositions. These uncertainties in simulated groundwater compositions may also be coupled to significant uncertainties in model predictions about how mineralogy, porosity, and permeability change over time.

Although uncertainty in simulated water compositions may be strongly dependent on the uncertainty in groundwater flow pathways, this is not always the case. Basic information about the chemical reactivity of rock layers within the model domain can provide useful insights about which types of new data may be most useful to collect, and which aspects of the model should be developed in more detail. For example,

- Accurate determination of infiltrating and initial water compositions is important when simulated groundwater flow occurs through chemically inert or slowly reacting rocks, because the water composition does not change significantly along the flow pathway.
- In contrast, efforts to explicitly model heterogeneities of the rock layers, lateral diversion, or matrix-fracture interactions, for example, will have little impact on geochemical predictions.
- When groundwater flow occurs through chemically reactive rocks, however, the opposite is true (i.e., initial and infiltrating water compositions are not important, but details of the groundwater flow pathway are).

References and Acknowledgements

References: Browning et al., Scientific Basis for Nuclear Waste Management XXIII. R. Smith and D. Shoesmith, eds. Symposium Proceedings 663, 2000 Browning et al., Computers & Geosciences special issue on "Reactive Transport Modeling in the Geosciences", 2003 (in press); Browning and Murphy (2002) CNWRA Letter Report; TDR-NBS-HS-000002 REV 00 ICN 02. CRWMS M&O. 2000. TDR-NBS-HS-000002 REV 00 ICN 02. CRWMS M&O. 2001. ANL-EBS-MD-000049, Revision 00, ICN02, North Las Vegas, Nevada.; Liu et al., Water Resources Research 34(10), pp. 2633-2646, 1998; Painter et al., CNWRA, 2001. Acknowledgements: This work is an independent product of the Center for Nuclear Waste Regulatory Analyses (CNWRA) and does not necessarily reflect the views or regulatory position of the U.S. Nuclear Regulatory Commission (NRC).