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U.S. Nuclear Regulatory Commission
ATTN: Mrs. Deborah A. DeMarco
Office of Nuclear Material Safety and Safeguards
Program Management, Policy Development, and Staff
Office of the Director
Mail Stop 8D–37
Washington, DC 20555

Subject: Programmatic Review of Poster

Dear Mrs. DeMarco:

The enclosed poster is being submitted for programmatic review. This poster will be submitted for presentation at the European Geophysical Society; American Geophysical Union; European Union Geosciences Conference, to be held April 4–13, 2002, in Nice, France. The title of the poster is:

"Reactive Transport Simulations of Alternative Flow Pathways in the Ambient Unsaturated Zone at Yucca Mountain, Nevada" by L. Browning, W. Murphy, C. Manepally, and R. Fedors

The presentation will discuss how uncertainties in ambient unsaturated zone flow pathways can lead to differences in simulated groundwater compositions and alteration mineralogies. Examples will be provided from MULTIFLO simulations of the ambient hydrogeochemical system at Yucca Mountain, Nevada, to illustrate how different types of couplings between geochemical and hydrological processes can impact uncertainties in reactive transport simulations.

This poster is a product of the CNWRA and do not necessarily reflect the view(s) or regulatory position of the NRC. Please advise me of the results of your programmatic review. Your cooperation in this matter is appreciated.

Sincerely yours,

Budhi Sagar
Technical Director

BS: ar
Enclosures

cc: J. Linehan, E. Whitt, B. Meehan, J. Greeves, W. Reamer, J. Schlueter, K. Stablein, J. Ciocco, H. Arlt, J. Bradbury, W. Ford, L. Hamdan, D. Brooks, A. Campbell, L. Campbell, B. Leslie, J. Schlueter, W. Patrick, E. Pearcy, L. Browning, C. Manepally, R. Fedors

Letter Only
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REACTIVE TRANSPORT SIMULATIONS OF ALTERNATIVE FLOW PATHWAYS IN THE AMBIENT UNSATURATED ZONE AT YUCCA MOUNTAIN, NEVADA

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Abstract

Chemical composition of groundwater can 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 the technical review of a potential application for the proposed nuclear waste repository at Yucca Mountain (YM), we evaluated the effect of alternative flow pathways on simulated groundwater compositions. This was accomplished by performing sensitivity studies on a calibrated reactive transport model for the ambient hydrogeochemical system at Yucca Mountain (Browning et al., 2003). Two alternative unsaturated zone (UZ) flow pathways were applied to the calibrated, base case model, and results of the 3 models were compared. All 3 models simulate two phase, non-isothermal, advective and diffusive flow and transport through one dimensional, matrix and fracture continua (dual permeability) containing at least 9 kinetically reactive hydrostatigraphic layers in the vicinity of the SD-9 borehole at YM.

Basic Model Properties (Cases 1-3)

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

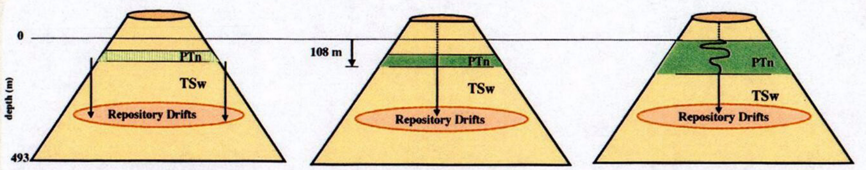
Gridding: a 56 cell structured grid with a mixed upper boundary condition (i.e. specified gas pressure, temperature and liquid flux) and a gravity drainage lower boundary condition.

Groundwater flow: Rock matrix and fracture networks in the unsaturated zone (UZ) are depicted as separate porous continua. Heat and 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

Geochemical Model: All 3 cases consider the following:
* 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.

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 (Table 1)
* 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 (Table 1)
* 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 (Table 1)
* Matrix-dominated flow in arbitrarily thick (120 m) section of PTn unit
* Fracture-dominated flow through TSw
* Travel time through PTn: 12,000 years

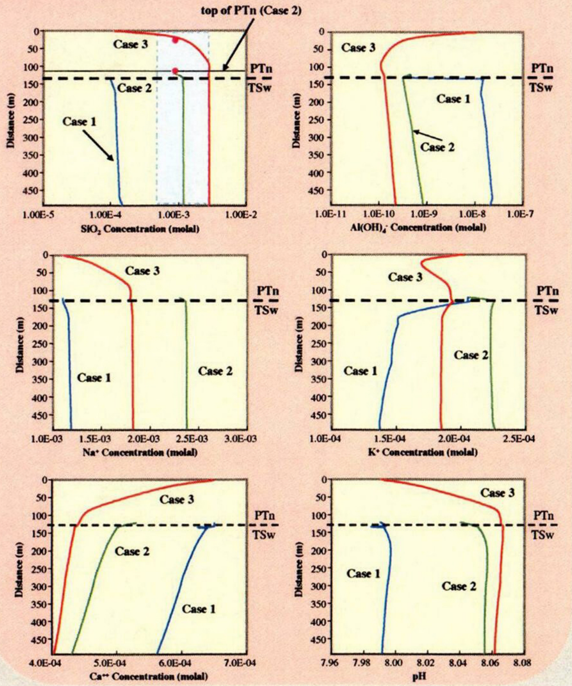
Groundwater Component	Colluvium (Cases 1 and 3)	[1]PTn Pore water (Case 2)
pH	7.99	8.04
Ca (mg/L)	14.00	22.7
Na (mg/L)	25	53
$SiO_2(aq)$ (mg/L)	5.8	48.6
K (mg/L)	8	8
Al (mg/L)	1.3e-5	1.3e-5
HCO_3^- (mg/L)	114.1	115.3
CO_3^{2-} (mg/L)	0.72	0.64
Cl (mg/L)	10.0	6.0

Table 1. Revised analytical matrix pore water compositions used to constrain boundary/initial conditions in our model

[1] Browning et al., 2000

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.



Discussion/Conclusions

Reactive Transport models are useful tools for predicting the potential effects of alternative flow pathways on simulated groundwater compositions. Our analyses illustrate the following relationships between ambient UZ flow pathways and simulated groundwater compositions under quasi steady state conditions:

In Reactive Units (e.g. PTn):

The longer the travel times for a packet of water through the unit, the greater the potential impact on simulated groundwater compositions (compare Cases 2&3).

The accuracy of simulated groundwater compositions in reactive units may depend strongly on how accurately the model represents heterogeneities in the horizontal thickness of the unit and/or the extent of lateral diversion.

The infiltrating groundwater composition may have no significant impact on simulated groundwater compositions (compare simulated SiO_2 concentrations, at 12 meters into PTn, Cases 2&3, as shown by magenta-colored circles)

Measured groundwater compositions can be useful for calibrating or validating geochemical models, but the simulated composition of percolating groundwater is controlled by water-rock-gas reactions.

In Unreactive or Slowly Reacting Units (e.g. most of the TSw):

The composition of infiltrating water has a stronger influence on simulated groundwater compositions than the thickness, direction, or length of the flow pathway within that unreactive unit.

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

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