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Scientific Notebook # 208

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Evolution of the Near-Field Environment
KTI
20-5708-561

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David R. Turner/Sr. Research Scientist . DRT

Objectives (20-5708-561) - KTI on Evolution of the Near-Field Environment (2/3/97)

The purpose of the research discussed in this scientific notebook is to evaluate available geochemical, geological, and hydrologic data in the vicinity of Yucca Mountainthat may have an impact on the evolution of the near-field environment. These data will be used to help provide site-specific constraints on reactive transport calculations and simulations of chemical changes in the near-field environment. The data will be based largely on pre-existing data acquired and/or compiled by the DOE and its contractors (e.g., USGS). Therefore, one of the main objectives of this scientific notebook is to document data sources and data quality (where possible). Another objective is to document assumptions and conditions used in setting up simulations using the MULTIFLO multicomponent, multispecies reactive transport code.

2/3/97 Mineralogy of Yucca Mountain

The following tables have been compiled in Excel, V.5.0 spreadsheet, including mineralogy determined using quantitative X-ray diffraction (XRD). The results have been obtained and reported in:

— Vaniman, D.J., D.L. Bish, S.J. Chipera, B.A. Carlos, and G.D. Guthrie, Jr. 1996 Summary and Synthesis Report on Mineralogy and Petrology Studies for the Yucca Mountain Site Characterization Project. Volume 1. Chemistry and Mineralogy of the Transport Environment at Yucca Mountain. US DOE, Milestone 3665

Unit contacts and depth to Water Table included in Vaniman et al (1996)

2/3/97 (DR)

2/3/97 (DR)

2/3/97 DRJ

2/3/97 DRJ

Order of mag
Ca for Gold
with moderate

2/3/97 DRJ

2/3/97 DRJ

2/3/97 DRJ

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2/3/97 DRK

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2/3/97 DRJ

2/4/97

Tpt = Topopah Spring tuff.

Total silica polymorphs = trid + crist + qz + opal-CT

Notes: ① Total silica is very constant across thickness of the Tpt. at about 40 wt%. Decreased over upper 45 m.

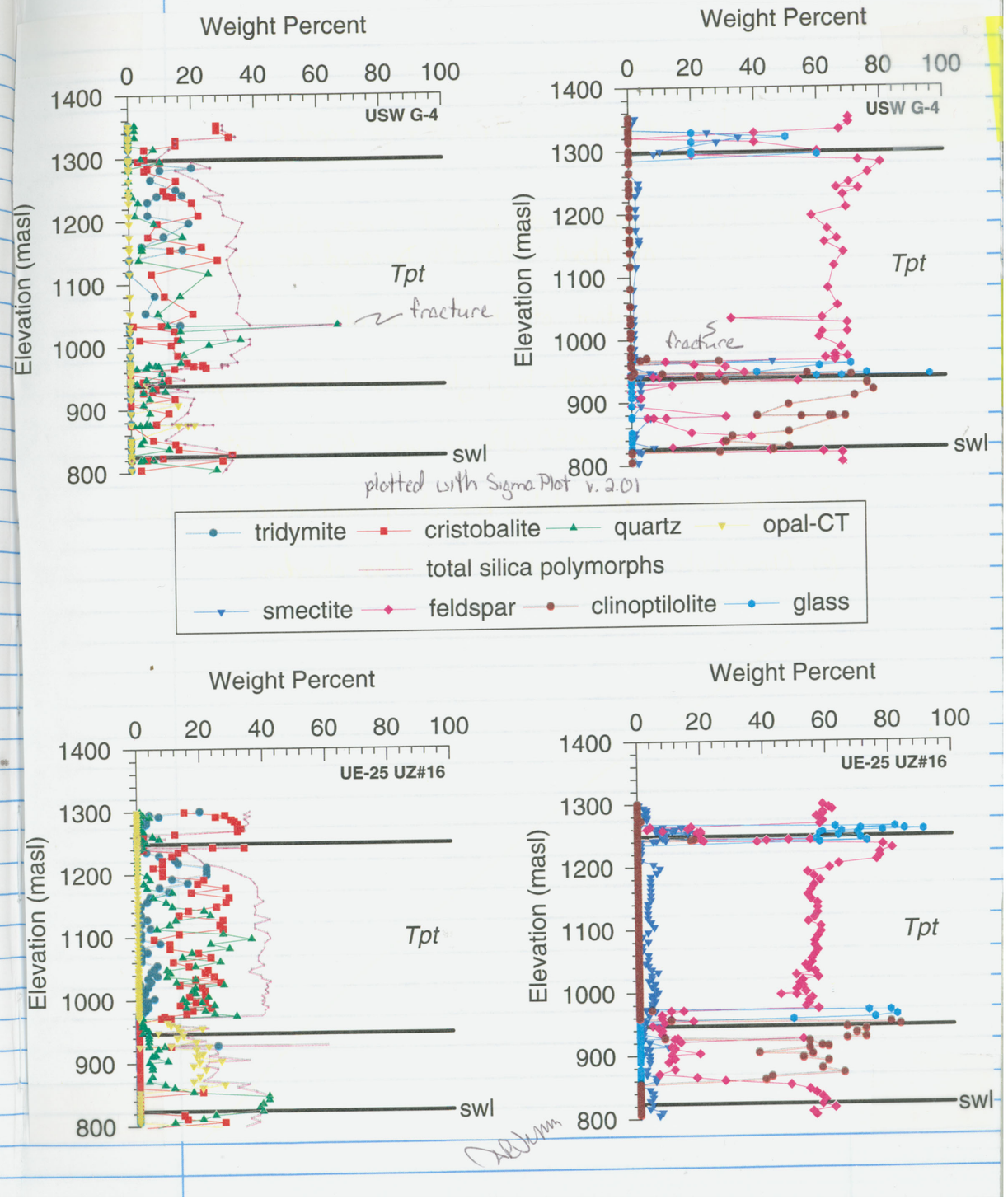
② Feldspar is constant at about 60-70 wt%.

③ Low Feldspar represents high glass near basal vitrophyre.

④ Feldspar jumps to ~80 wt% over upper 45 m of Tpt.

⑤ Clinoptilolite limited to below base of Tpt and static water level

⑥ Clinoptilolite inversely related to feldspar abundance.



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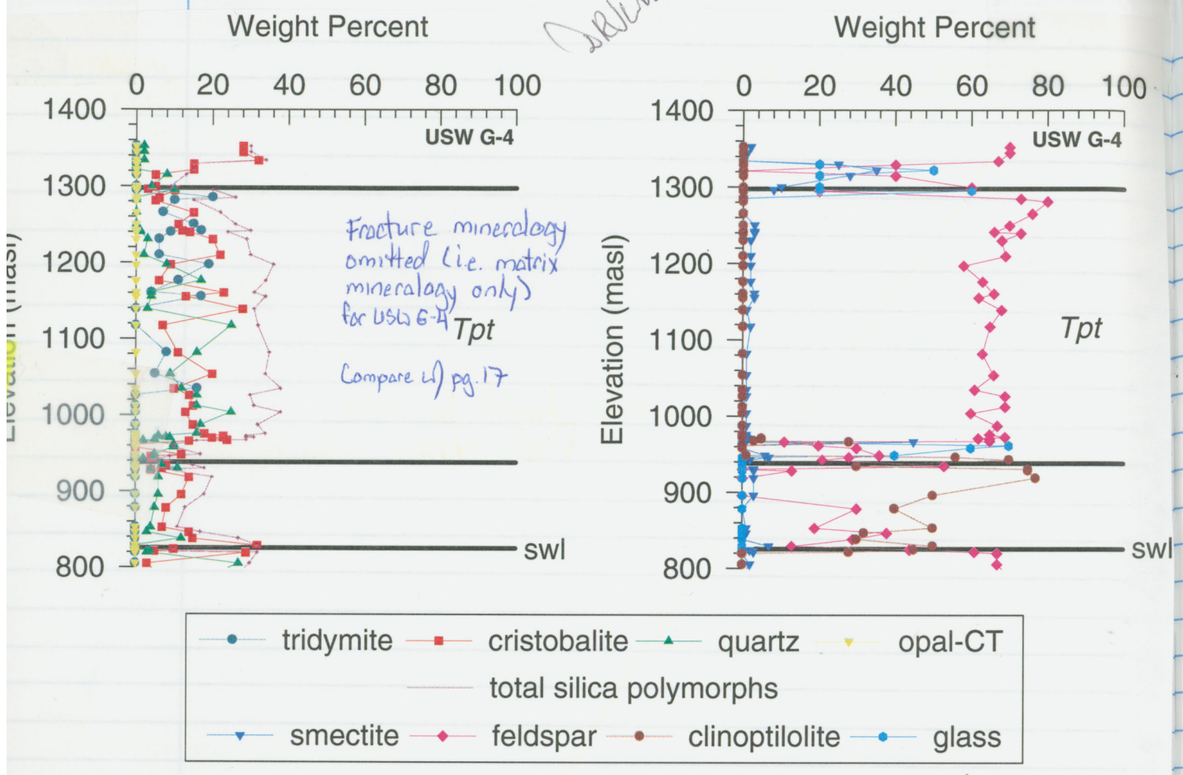

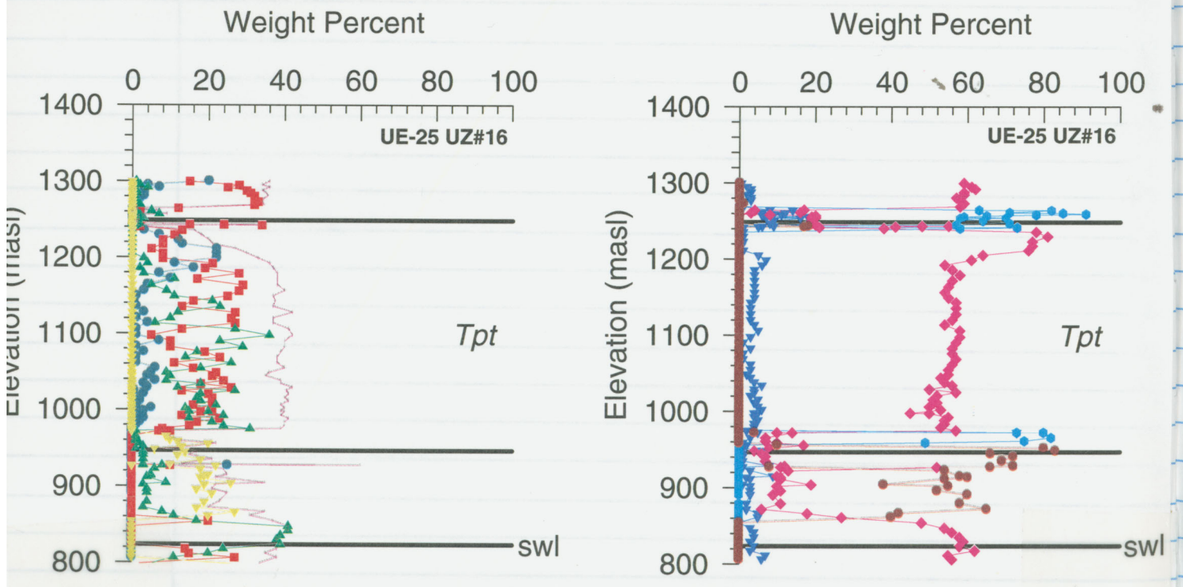

TPA sensitivity analyses:

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Page should be blank DRJ 10/22/97 - see pg. 21

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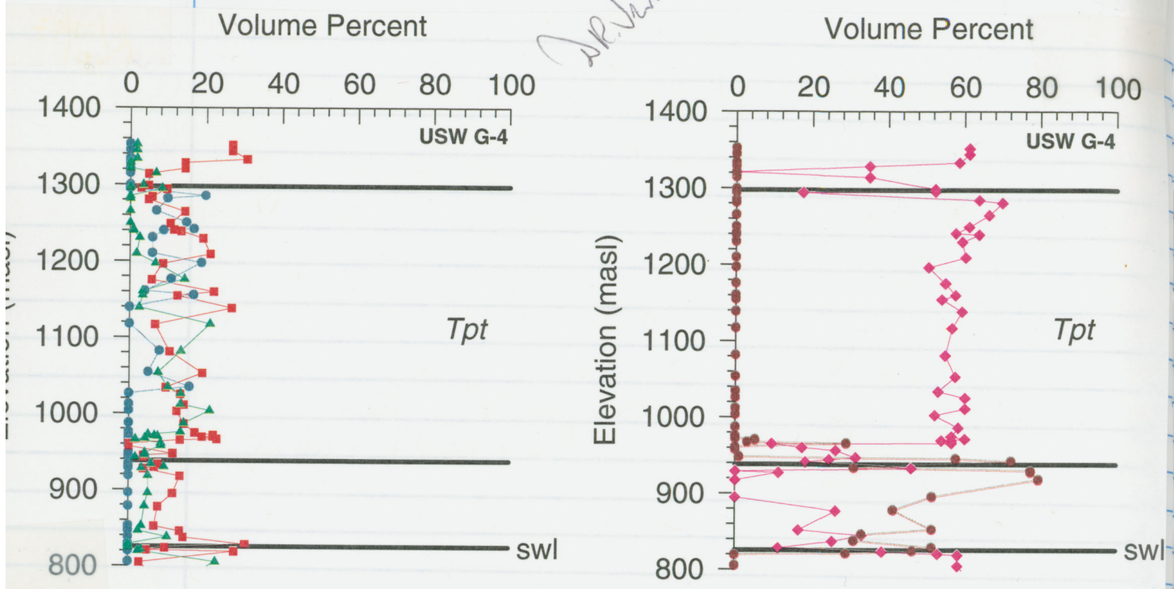
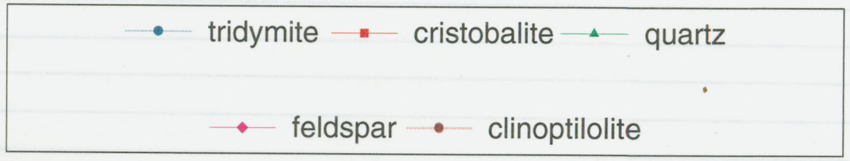
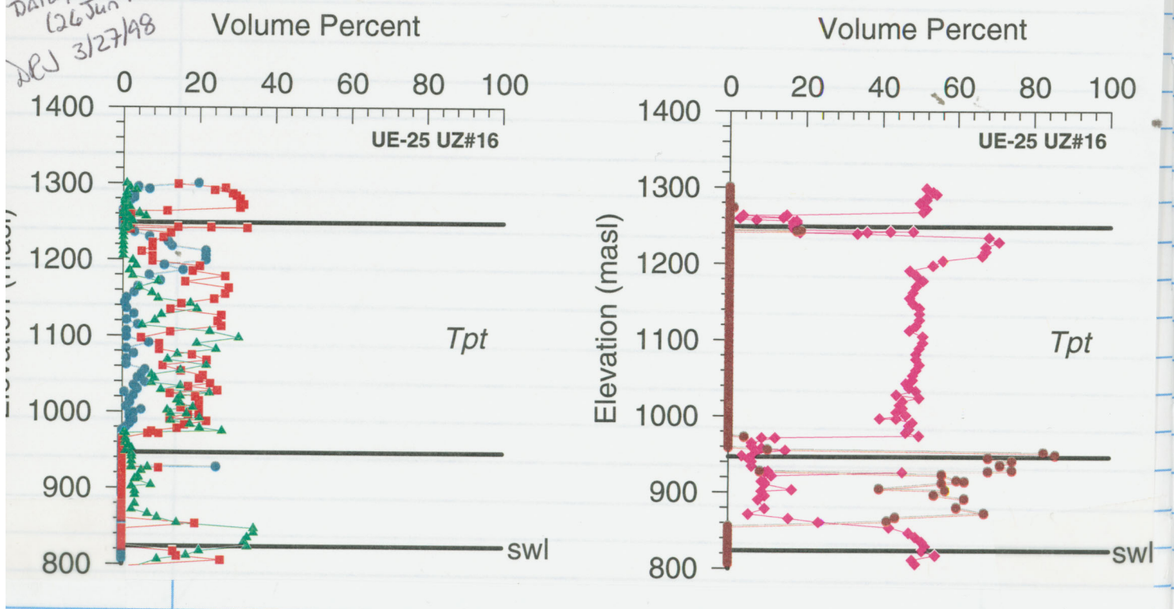




Molar Volume for Cpt + Mont from EQ3/6 data0.com.r16 (26 Jun 92) DBJ 3/27/98



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Iron Oxyhydroxide Pseudocolloid Scenario-Basis for Modeling Approach

To simulate the extent of the near-field, the transport of pseudocolloids is limited to the Topopah Spring tuff. Because of large uncertainties in estimating the amount of colloid-size iron oxyhydroxide generated by waste package degradation, possible effects on solubility or increased loading to levels in excess of solubility limits is not considered. In addition, the possibility of plugging fractures and matrix porosity by particulates is acknowledged, but is not specifically considered here. It seems likely that effects on hydrologic parameters in the near-field due to iron oxyhydroxides will be overshadowed by those induced by cement-water interaction.

Of the elements currently considered in the TPA database, not all are likely to sorb strongly onto iron oxyhydroxides to form pseudocolloids. Those not considered in this analysis are Tc-99, I-129, C-14, Cl-36, and Cs-135. It is possible that the anions Cl and I will sorb on iron, but there is no available data. In addition, anion sorption may be greatly reduced at high pH values possible in the near-field. For Tc, the effect of iron will be more significant in helping to reduce Tc(VII) to Tc(IV), with lower solubility and increased sorption, but there is a lack of data to estimate Tc sorption behavior. Similar to Na, Cs is a weakly hydrolyzable cation and is not likely to interact strongly with iron. Carbon has been shown to sorb onto iron oxyhydroxide, but the effect is probably small relative to the effects of carbonate precipitation/dissolution.

Basis for Parameter Values

Two conceptual models can be considered simultaneously:

- Colloid transport through fractures. Fracture apertures in the Topopah Spring are on the order of 100 microns and larger (Wilson et al., 1994), and may be large enough to transport colloids (< 1 micron). For this scenario, the Fracture Retardation Factor (R_d) can be modified. The principal concern with colloid transport is the possibility of unretarded transport and possible early breakthrough due to hydrodynamic forces. Because the TPA code already assumes no retardation in fractures (i.e., R_d=1.0), the only consideration is enhanced transport (R_d<1).

  A lack of experimental data make it difficult to constrain the impact, if any, of this effect on radionuclide transport. In the absence of any definitive estimates of colloid transport, a maximum of 10 percent enhancement of fracture colloid transport is assumed. Since only iron oxyhydroxide pseudocolloids are considered here, the same distribution (uniform) is assumed for all radioelements (Table 1).

Table 1. Fracture retardation coefficients (unitless) for the TSw.

Radionuclide	Fracture Retardation (R_d)					
	Current Values (tpa.inp.meanvalues)		Proposed Values			
	Distrib.	Value	Distrib.	Min	Max	Mean
Am-241	Constant	1.0	uniform	0.90	1.0	--
Am-243	Constant	1.0	uniform	0.90	1.0	--
Cm-246	Constant	1.0	uniform	0.90	1.0	--
Cm-245	Constant	1.0	uniform	0.90	1.0	--
Nb-94	Constant	1.0	uniform	0.90	1.0	--
Ni-59	Constant	1.0	uniform	0.90	1.0	--
Np-237	Constant	1.0	uniform	0.90	1.0	--
Pb-210	Constant	1.0	uniform	0.90	1.0	--
Pu-240	Constant	1.0	uniform	0.90	1.0	--
Pu-239	Constant	1.0	uniform	0.90	1.0	--
Ra-226	Constant	1.0	uniform	0.90	1.0	--
Se-79	Constant	1.0	uniform	0.90	1.0	--
Th-230	Constant	1.0	uniform	0.90	1.0	--
U-238	Constant	1.0	uniform	0.90	1.0	--
U-234	Constant	1.0	uniform	0.90	1.0	--

Colloid filtration by the pores of the matrix and enhanced retardation by the iron oxyhydroxides relative to the tuff mineralogy. A specific filtration mechanism (chemical attachment, straining) is not implied. Two populations of pore sizes cluster around five and 200 microns (Peters et al., 1984). This may be large enough to transport colloids, but the likelihood of constricted pore throats and slow matrix flow suggest that colloid transport through the matrix is limited. This is consistent with field observations at the Peña Blanca site where higher uranium concentrations are associated with hematite in fractures, and uranium migration into the matrix is limited. Matrix sorption coefficients (K_d) values are assumed for each of the radioelements for the Topopah Spring tuff (Table 2). For the purposes of the sensitivity analysis, the K_d distribution developed through expert elicitation for TSPA-93 (Wilson et al., 1994) will be used to identify

Table 2. Matrix sorption coefficient (K_d) values assumed for the TSw. (from TSPA-93. Wilson et al, 1994).

Radionuclide	Matrix K_d (m^3/kg)					
	Current Values (tpa.inp.meanvalues1)		Proposed Values			
	Distrib.	Value	Distrib.	Min	Max	Mean
Am-241	constant	0.81	uniform	1.0	5.0	--
Am-243	constant	0.81	uniform	1.0	5.0	--
Cm-246	constant	0.45	uniform	1.0	5.0	--
Cm-245	constant	0.45	uniform	1.0	5.0	--
Nb-94	constant	0.0	uniform	1.0	5.0	--
Ni-59[a]	constant	0.0037	logtriangular	0.003	1.0	0.9
Np-237	constant	0.0045	uniform	0.5	1.0	--
Pb-210	constant	0.0068	uniform	0.1	1.0	--
Pu-240	constant	0.17	uniform	1.0	5.0	--
Pu-239	constant	0.17	uniform	1.0	5.0	--
Ra-226[b]	constant	1.5	triangular	0	0.75	0.03
Se-79	constant	0.0026	uniform	0.1	1.0	--
Th-230	constant	0.048	uniform	1.0	5.0	--
U-238	constant	0.0002	uniform	0.1	1.0	--
U-234	constant	0.0002	uniform	0.1	1.0	--

a. Ni-59 is given a log beta distribution in TSPA-93, and due to limitations of LHS, is approximated by a logtriangular distribution.

b. Ra-226 given a beta distribution in TSPA-93, and due to limitations of LHS, is approximated here as a triangular distribution.

the minimum, maximum (and mean if appropriate) K_d for iron oxyhydroxides. Curium was not considered in TSPA-93; due to its 3+ valence, however, Cm is assigned the same K_d distribution as Am and Nb.

Results

The TPA input file tpa.inp.meanvalues1 was modified to reflect the values and distributions given in Tables 1 and 2. In the simulations, 220 realizations (equal to 10n for n=22 variables) were run for 10,000 years at five kilometers. Both R_d and K_d were allowed to vary during the simulation. Results showed that for all radionuclides considered, time-to-peak dose, peak dose, and release from the unsaturated zone to

the saturated zone were unaffected by variations in TSw R_d and K_d values. Results were identical for each of the 220 realizations for each radionuclide. Additional interpretation of the results are necessary to determine the cause for this insensitivity.

Conclusions

Colloid transport through the unsaturated zone is poorly characterized, and many assumptions used here are not well supported. Because of the abstractions used in TPA, there are many limitations to applying the current code to colloid transport. For example, TPA does not allow for partitioning between a colloid and a dissolved aqueous phase, The current model does not consider competitive sorption between a colloidal phase and the tuff minerals, and fracture transport does not specifically consider iron oxyhydroxide transport. Also, the total amount of colloid material likely to be present in the near field is not explicitly considered. It is therefore implicit in the conceptual model that all transport in the fractures occurs as colloids and that the transport properties of the iron oxyhydroxides controls radionuclide migration through the matrix. In addition, as discussed above, the current conceptual model is only designed to address to colloid transport. Other potential effects of colloids such as releases exceeding solubility limits or plugging of fractures and pores are not explicitly considered here. Future studies may focus on these effects.

The distributions assumed for matrix K_d values are based on the informal expert elicitations used in TSPA-93 (Wilson et al., 1994). A more detailed model such as a surface complexation model could be used in a limited sense to further constrain likely sorption coefficients for the chemical conditions expected at Yucca Mountain.

In the current model, iron oxyhydroxide is the only sorptive mineral specifically considered (only for matrix sorption). For this reason, retardation and sorption behavior should be strongly correlated between different radionuclides. The current version of the TPA code does not, however, allow for correlations between retardation factors or sorption coefficients. Therefore, selecting a distribution with a mean and maximum is best considered as a first approximation. Future consideration in TPA of pseudocolloid formation (and sorption behavior as well) should be modified to include a correlation among sorption coefficients.

Finally, only the Topopah Spring tuff is considered in the near-field. While this is the first unit that any colloids released from the repository will have to pass through, colloid transport may be very different in other units due to differences in fracturing and porosity.

References

Peters, R.R., E.A. Klavetter, I.J. Hall, S.C. Blair, P.R. Heller, and G.W. Gee. 1984. *Fracture and Matrix Hydrogeologic Characteristics of Tuffaceous Materials from Yucca Mountain, Nye County, Nevada.* SAND84-1471. Albuquerque, New Mexico: Sandia National Laboratories.

Wilson, M.L., J.H. Gauthier, R.W. Barnard, G.E. Barr, H.A. Dockery, E. Dunn, R.R. eaton, D.C. Guerin, N. Lu, M.J. Martinez, R. Nilson, C.A. Rautman, T.H. Robey, B. Ross, E.E. Ryder, A.R. Schenker, S.A. Shannon, L.H. Skinner, W.G. Halsey, J.D. Gansemer, L.C. Lewis, A.D. Lamont, I.R. Triay, A. Meijer, and D.E. Morris. 1994. *Total System Performance Assessment for Yucca Mountain - SNL Second Iteration (TSPA-1993).* SAND93-2675. Albuquerque, NM: Sandia National Laboratories.

This notebook appears to comply with QAP-003.

P. C. [illegible]

2/3/2000