AN UPDATED SITE SCALE SATURATED ZONE GROUND WATER TRANSPORT MODEL FOR YUCCA MOUNTAIN

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This paper summarizes the numerical site scale model developed to simulate the transport of radionuclides via ground water in the saturated zone beneath Yucca Mountain.

I. INTRODUCTION

The U.S. DOE has submitted a license application to the Nuclear Regulatory Commission (NRC) to create a geologic repository at the Yucca Mountain, Nevada (Figure 1), for the disposal of spent nuclear fuel and high-level radioactive waste. A number of engineered and natural barriers are expected to retard any potential release of radionuclides from the repository and to reduce their concentrations. In the event of a release, the ground water beneath the Yucca Mountain is a primary medium through which most radionuclides might move from the geologic repository to the accessible environment at the compliance boundary. The role of the saturated zone (SZ) is to delay the transport of radionuclides to the accessible environment and to reduce the concentration of radionuclides before they reach the accessible environment. Radionuclide breakthrough curves are determined by the specific discharge, flow paths and flow distribution of ground water, and the mechanisms of solute transport including advection, dispersion, diffusion, sorption and colloid-facilitated transport. This paper describes the development of a site scale transport model to evaluate these processes.

II. FLOW MODEL

Yucca Mountain is located about 150 km northwest of Las Vegas, Nevada (Figure 1) in the Great Basin section of the Basin and Range province[1]. Yucca Mountain consists of a group of north-trending block-faulted ridges composed of volcanic rocks bounded by basins composed of volcanic tuffs, which pinch out to the south beneath valley-fill alluvium, underlain by a thick carbonate aquifer. In general, the confining units are zeolitic, nonwelded tuffs and the aquifers are welded, fractured tuffs.

The conceptual model of SZ flow in the model area is that ground water flows generally southwards from recharge areas to the north and at higher elevations, through the volcanic rocks towards the Amargosa Desert [2]. Towards the southern portion of the model area, the flow near the water table enters the valley-fill alluvium. Data suggests an upward gradient indicating that, for the immediate Yucca Mountain area and downstream, radionuclide transport would be restricted to the volcanic and alluvial formations. Discharge from the model occurs mainly via the alluvium, at the model boundary to the south and southeast, and through pumping out of wells in the Amargosa Valley.

The overall groundwater system is assumed to be in steady state for the purpose of this modeling. A confined aquifer solution is used for the flow model. The top boundary of the model represents the observed water table levels. The effective continuum approach is used to model flow and transport, which averages fracture and surrounding rock properties in a given grid block, with the modification that several of the important fault zones are included as explicit features[2].

The flow and transport modeling is done with the FEHM computer code[13], a general purpose unsaturated-saturated zone non-isothermal code built around state-of-the-art control volume finite element numerical procedures. Solute transport is simulated using a particle tracking technique with a generalized dispersion tensor that allows for different longitudinal dispersivities in the vertical and the horizontal directions, matrix diffusion, and sorption.

The site scale flow model is a rectangular area about 30km east west and 45 km north south including the Yucca Mountain[2]. The geometry of geologic units was defined in a hydrogeologic framework model (HFM2006) with 27 hydrologic units constructed using data such as geologic maps and sections, borehole lithologic logs, and topographic digital elevation models[3]. Major hydrogeologic features such as fault zones, and areas of hydrogeologic alteration were classified as distinct permeability zones.

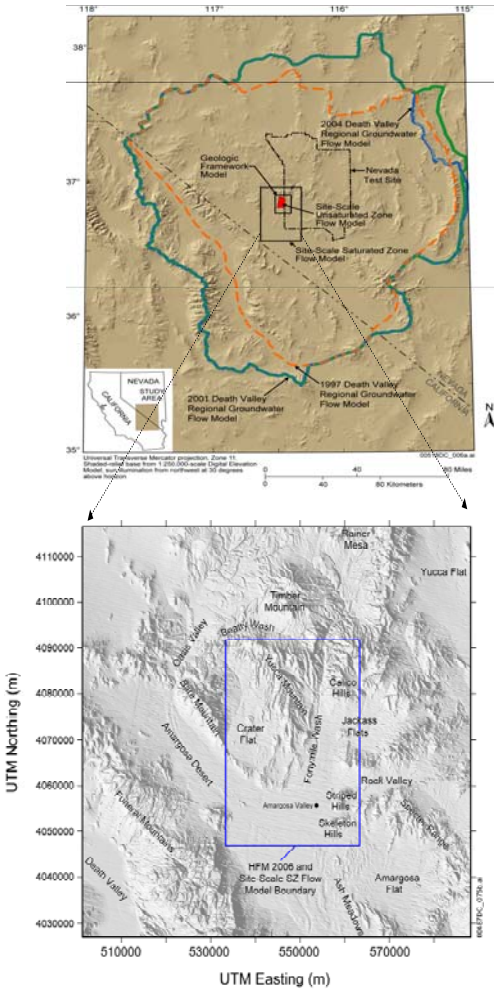

Fig. 1: Location Map Of The Yucca Mountain Project And An Enlargement Showing The Saturated Zone Study Area And Associated Geological Features.

A structured computational grid (Figure 2) was created from the HFM2006 with uniform horizontal 250 m grid spacing. The vertical grid spacing ranges from 10 m at the upper boundary near the water table to 600 m deep within the SZ.The vertical grid extends from an elevation of +2018.5 m to –4000 m (MSL). The permeabilites of various units in the model were optimized using a parameter estimation code (PEST) to achieve a minimum difference between observed water levels and simulated water levels, and also between volumetric/mass flow rates along specific boundary segments simulated by the SZ regional- and site-scale models. Post-development model validation[2] was accomplished by comparing a) predicted hydraulic heads with new water-level data, b) predicted flow paths with those estimated from hydrochemistry and isotope data, c) calibrated parameter values with those derived from well testing, and d) predicted specific discharge with the conclusions of the Expert Elicitation Panel[4].

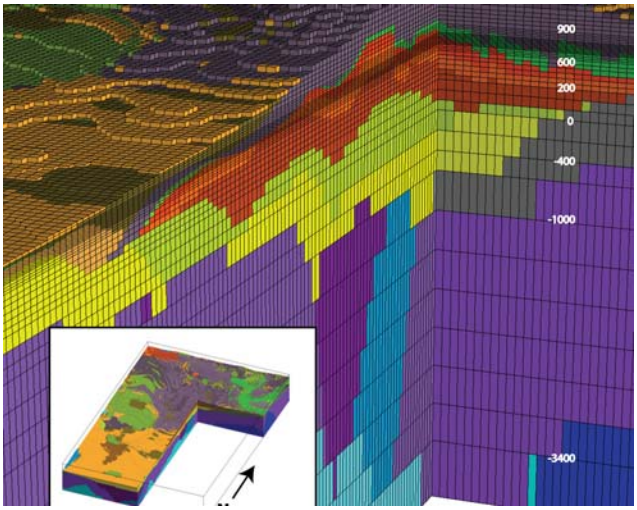

Fig. 2: Close-Up View of Computational Grid (3× Vertical Exaggeration) Showing Cut Away at UTM Easting = 549,000 m and UTM Northing = 4,078,000 m Through the Yucca Mountain Repository.

III. TRANSPORT MODEL

Radionuclides are modeled to enter the SZ via downward percolation of water from the unsaturated zone. Within the SZ model, radionuclides are transported in the upper few hundred meters below the water table with pore water that flows sub-horizontally in a southwardly direction through the highly fractured portions of the tuff, entering the alluvium to the south. Current hydrologic evidence supports the model of fluid flow within fractures in the moderately to densely welded tuffs of the SZ[5]. Fluid flow within fractures occurs preferentially along tortuous channels of largest aperture, with stagnant fluid residing in the low permeability rock matrix. Diffusion of solutes between the stagnant water in the rock matrix and the flowing fracture zones is simulated using a dual-porosity approach for the volcanic formations. In the alluvium, flow and transport is represented using a single porosity continuum model. This is due to the more porous, less fractured nature of the alluvial material. Alluvium is a heterogeneous medium, flow occurs through the relatively more permeable regions within the medium, with the low-permeability regions acting as flow barriers that groundwater flows around rather than through.

Dispersion is caused by heterogeneities at all scales, from the scale of individual pore spaces to the scale of the thickness of individual strata and the length of structural features such as faults. The spreading and dilution of radionuclides that result from these heterogeneities could

be important to performance of the potential repository. The largest heterogeneities are represented explicitly in the site-scale SZ flow and transport model[2]. For dispersion at smaller scales, it is assumed that the convective-dispersion model applies with dispersion characterized using an anisotropic dispersion coefficient tensor consisting of longitudinal, horizontal-transverse, and vertical-transverse dispersivities[7].

Field studies of transport and dispersion have been conducted at a variety of length scales (from meters to kilometers) to address the issue of dispersion. The results show a trend toward larger apparent dispersion coefficients for transport over longer distances. Solutes encounter larger-scale heterogeneities at larger scales, and thus, spreading is more pronounced. The dispersivity estimates from C-wells tracer experiments fall within the range of values from other sites[7], suggesting that transport in the fractured tuffs exhibits similar dispersive characteristics. The values used in the simulations of radionuclide transport are somewhat higher than those estimated from the C-wells because of the larger scale that is relevant for radionuclide migration to the accessible environment. Transverse dispersion is conservatively assigned a very low value in the transport model.

Because the site-scale SZ flow and transport model is used to predict transport under a well-withdrawal scenario[8], the potentially complex distribution of radionuclides within a grid block will be averaged in the process of extracting water from the aquifer.

Sorption of radionuclides on rock surfaces is a mechanism that will enhance retardation of the solute movement. Radionuclide-rock interactions potentially can occur on the surfaces of fractures and within the rock matrix. Sorption within the rock matrix is supported by the C-wells tracer experiments[9]. As a conservative approach, sorption on fracture surfaces is not included in the model.

Sorption reactions are represented in the transport model by a constant sorption coefficient (k_d), which is the ratio of the solute adsorbed on the solid to that in solution . The values of these k_d's are sensitive to the radionuclide element being considered and geological variables including rock type, water chemistry, redox condition of the ground water, radionuclide concentrations, and variations in rock surface properties within the major rock types [7]. As a conservative approach, the groundwater was assumed to be in oxidizing conditions. Since there is uncertainty in knowledge regarding the geological variables, probabilistic uncertainty distributions were developed for each radionuclide of interest. The distributions selected were based in part on laboratory data and in part on professional judgment regarding the impact of variables not considered in the experimental program. The experimental data were augmented with the results of modeling calculations using the code PHREEQC[10] to provide a basis for interpolation and extrapolation of the data.

The use of a k_d to represent sorption reactions in a transport calculation requires that the sorption reaction be reversible, linear (isotherm) and instantaneous. On the time scale of radionuclide transport from a repository, these criteria will generally be met[7]. The probability distributions of k_d's are biased towards lower values to compensate for any nonlinear sorption.

Transport of radionuclides via colloids is another mechanism that is of importance at field scale[11]. Solute molecules can absorb onto the colloid particles and be transported along with them. Because the colloidal particles are much larger in size and mass than the radionuclides that sorb onto them, the radionuclides do not affect the transport of the colloid particles. The colloids in the saturated zone can be of several types including natural colloids (typically clay or silica), waste-form colloids resulting from degradation of spent nuclear fuel or glass, and iron-oxyhydroxide colloids resulting from degradation of the waste container[11]. Because of the relatively large size of the colloids, matrix diffusion of these particles is negligible. Several field observations have suggested that a small percentage of colloids has the potential to transport unretarded with groundwater[12], whereas the majority undergo filtration, which can be described by a retardation factor, which is the ratio of the travel time including filtration to that without filtration..The retardation factor is dependent on several factors such as colloid size, colloid type, and geochemical conditions (e.g., pH, Eh, and ionic strength).

A fraction of the total radionuclide inventory (1% to 10%)[11] is expected to reach the SZ as radionuclides that attach reversibly to the colloids, thus partitioning their transit time between the solution, attached to the rock walls, and attached to the colloids. The radionuclides that are reversibly absorbed onto colloids are modeled using the K_c model. K_c (groundwater concentration of colloids times sorption coefficient onto colloids) represents the equilibrium partitioning of radionuclides between the aqueous phase and the colloidal phase with the distribution coefficient[7]. In this approach the diffusion coefficient and the sorption coefficient for the radionuclide are reduced to account for the fraction of time spent by the radionuclide attached to the colloid particles. The distribution coefficient K_c is modeled as a function of radionuclide sorption properties, colloid substrate properties, aqueous chemistry, and colloid concentration, but independent of the properties of the immobile media through which transport occurs. The radionuclides that are irreversibly absorbed onto the colloids are modeled to transport in a manner identical to the colloids onto which they are sorbed.

A site scale transport model was built on the basis of the site scale flow model using particle tracking and incorporating matrix diffusion, dispersion and sorption.

The flow paths and travel times are found to agree with the regional geochemistry data[2], providing additional confidence in the transport model. The ^{14}C ages for water samples from wells within the site scale model domain range from about 11430 years to 16390 years[2], which compare well with the model predictions[7].

VI. MODEL UNCERTAINTIES

Model form uncertainty in regards to the transport model is explicitly addressed by discussing alternative conceptual models. Although the base case model is designed to accurately represent the saturated zone transport, the transport model was selected such that it resulted in transit times faster than those expected using alternative conceptual models. Certain alternate conceptual models were accommodated within the current mathematical model framework by modifying the uncertainty distributions of the effective parameters.

Certain alternative conceptual models lead to transit times greater than the base-case results and were not included in the transport model. These were[7]: 1) the matrix material intervening the fracture zones in volcanics permits significant fluid flow, 2) radionuclides undergo irreversible sorption on the rock surfaces, 3) radionuclides precipitate forming solid rock phases, 4) water table rises due to future climate changes, and 5) solutes diffuse into low permeability zones in alluvium.

The alternative conceptual models implicitly included in the site-scale saturated zone transport model by modifying the uncertainty distributions of the effective parameters were[7]: 1) sorption reactions are not instantaneous, 2) sorption reactions are non-linear, 3) sorption parameters vary locally within the model domain, and 4) in alluvium, high-permeability channels exist that can provide preferential pathways for flow and transport.

V. TRANSPORT PARAMETERS

The input parameters of importance to the transport model, along with the range of values for each are presented in Table 1. Uncertainty in regards to the values of transport model is unavoidable given the sparseness of observed data and the limited amount of information available. Much of the data used for deriving parameter values are from experiments conducted on spatial and temporal scales much smaller than those in the site scale SZ model. Hence uncertainty ranges and distributions for the various transport parameters were developed[7] on the basis of available data from site specific field experiments, laboratory measurements on drill-cuttings and core samples obtained from the site, well logs, relevant data from other sites, and expert elicitation. The details of the basis of development of these uncertainty distributions are presented elsewhere[14]. The base case transport model presents the case of non-sorbing radionuclides. Base-case values for most parameters were chosen to be the median values for the distributions except for sorption related parameters.

TABLE 1. Input Parameters and Range of Values[7] for the Site-Scale Saturated Zone Transport Model

Parameter	Base-Case (Stochastic Uncertainty Range)	Parameter	Base-Case (Stochastic Uncertainty Range)
Specific discharge multiplier	1 (0.112 to 8.933)	**Permeability horizontal anisotropy ratio (N-S/E-W)**	5 (0.05 to 20)
Bulk density in alluvium	1910 (1669 to 2151) kg/m^3	**k_d in alluvium**	0.0 [b] (0 to 10^4) mL/g
Effective porosity, alluvium	0.18 (0.02 to 0.3) fraction	**Colloid retardation factor in alluvium**	1 [b] (8 to 5195)
Flowing interval porosity	0.001 (10^{-5} to 0.1) fraction	**Flowing interval spacing**	25.773 (1.86 to 80) m
Matrix porosity in volcanics	0.15 – 0.25 [a] fraction	**Diffusion coefficient in volcanics**	5.0×10^{-11} $5.0 \times (10^{-12}$ - $10^{-10})$ m^2/s
Matrix sorption coefficient in volcanics	0 [b] (0 to 10,000) mL/g	**Colloid retardation factor in volcanics**	1 [b] (6 to 794)
Groundwater concentration of colloids	0 [b] (10^{-9} to 2×10^4) g/mL	**Sorption coefficient onto colloids**	0 [b] (1 to 1.0×10^7) mL/g
Unretarded fraction of colloids	0 [b] (0.00034 to 0.0017)	**Dispersivity, longitudinal**	10 (0.1 to 2000) m
Dispersivity, transverse, horizontal	0.05 (0.0005 to 10) m	**Dispersivity, transverse, vertical**	0.0005 (5×10^{-6} to 0.1) m

[a] this parameter is not treated stochastically in the TSPA, but assigned fixed values that differ on a unit by unit basis

[b] base case value represents non-sorbing radionuclides.

VI. RESULTS

A plan view of the particle tracks for nine particles with starting locations distributed over the repository footprint are shown in Figure 3, along with flow paths deduced from geochemistry data[2]. A good agreement is noted between the two sets of flow paths. The base case (Table 1) serves as a reference point for exploring the role of processes and features of the system in subsequent simulations. The particle source location was chosen near the middle of the repository footprint at the water table. Calculations were performed for an instantaneous release of particles at the source location.

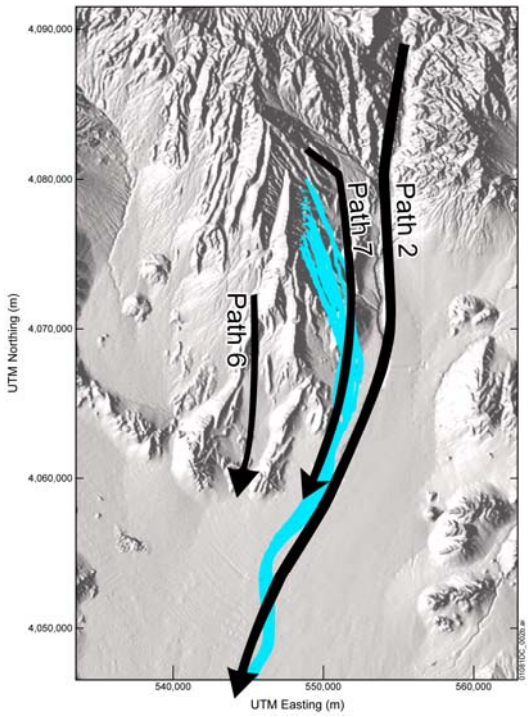

Fig. 3 Particle Tracks Resulting From The Site-Scale Saturated Zone Base-Case Transport Model (In Blue), Compared Against The Transport Pathways Deduced From Hydrochemistry Data (In Black).

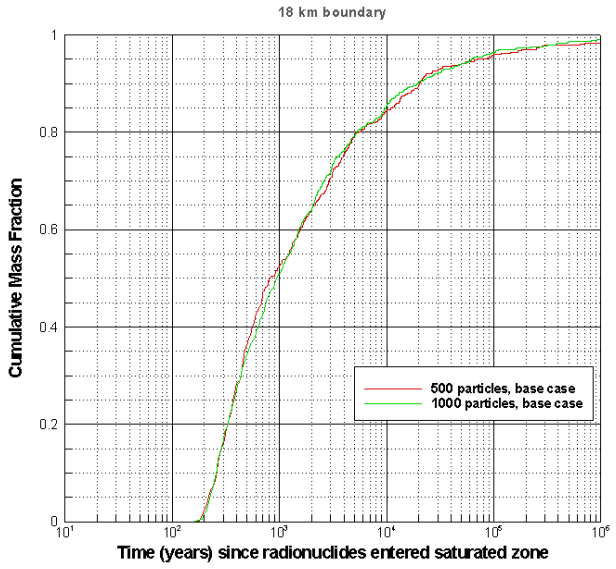

Fig. 4. Breakthrough Curves At The 18-Km Boundary For The Transport Base Case (500 Particles For A Conservative, Nonsorbing Radionuclide) With 1000 Particle Case For Comparison.

The BTC at the boundary of the accessible environment at 18 km was calculated by releasing 500 particles and by outputting the cumulative number of particles crossing an east-west vertical plane across the entire width and depth of the model. This is the BTC for a conservative, nonsorbing radionuclide in the absence of radioactive decay. Breakthrough times on the order of hundreds of years are predicted for the bulk of the mass arriving at the water table, with transport times extending into thousands of years for the slowest moving 20% of the mass. The time for 50% of the initial mass to breakthrough at the 18km compliance boundary (BT) for the curve in Figure 4 is 810 years. For comparison, also shown in Figure 4 by the green curve is the BTC for base case with initial number of particles being 1,000 instead of 500. As expected, although this curve is smoother than the BTC for 500 particles, they compare well with each other.

The results from simulations that evaluate the effect of changes in the specific discharge are shown in Figure 5. In these simulations, the base-case flow model was modified to scale the input recharge fluxes by the same factor as the rock permeabilities to preserve the model calibration. The results show the sensitivity of the output to the level of uncertainty in this parameter. For the case of upper limit of specific discharge multiplier where the base-case fluxes are multiplied by a factor of 8.933, BT is 31 years (with extremely fast fluid flow such as would be expected for the very unlikely case of a high-permeability channel going continuously over the distance of 18 km in a highly faulted region). The lower limit of specific discharge multiplier, a factor of 0.112, leads to a BT of 52,840 years.

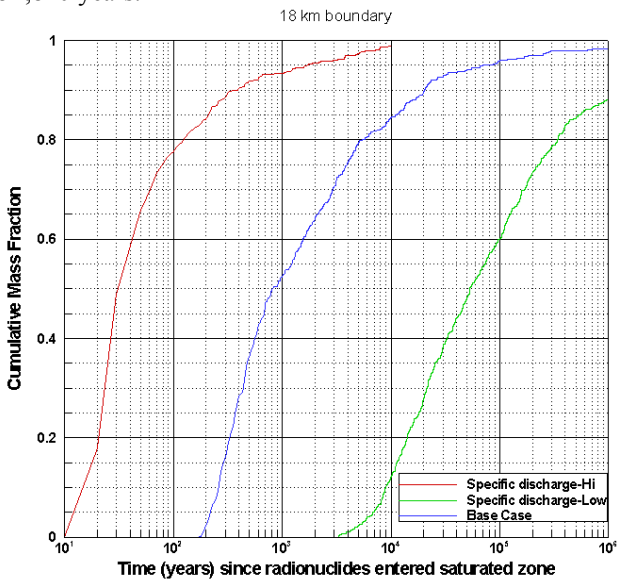

Fig. 5. Propagation of Input Uncertainty in the Specific Discharge to the Output Breakthrough Curves at the 18-km Boundary.

The results from simulations that evaluate the effect of changes in effective diffusion coefficient in volcanics on the BTCs are shown in Figure 6. Also shown in the

figure for comparison is the BTC for practically zero diffusion (diffusion coefficient of 10^{-50} m^2/s). The range of 5.0×10^{-12} to 5.0×10^{-10} (m^2/s) in the input value results in the range of 245 to 6,324 years for BT. Note that this parameter affects only transport through the volcanics and not through the alluvium.

Figure 7 shows two simulations of sorbing radionuclides. The curve labeled "Matrix sorption" allows sorption in the matrix continuum of the volcanic tuffs and reflects a small matrix sorption coefficient of 1.3 mL/g. Including only this process yields a BTC similar to the base-case BTC but with significantly delayed transport times. The final curve in the figure shows the influence of sorption in the alluvium along with the fractured volcanics. Travel times largely in excess of 10,000 years are predicted in the saturated zone alone for a sorption coefficient of 6.3 mL/g, a value meant to fall in the range of k_d values for weakly sorbing radionuclides such as neptunium. As seen from these curves sorption in the alluvium can increase the transport time by orders of magnitude for even the weakly sorbing radionuclides such as neptunium.

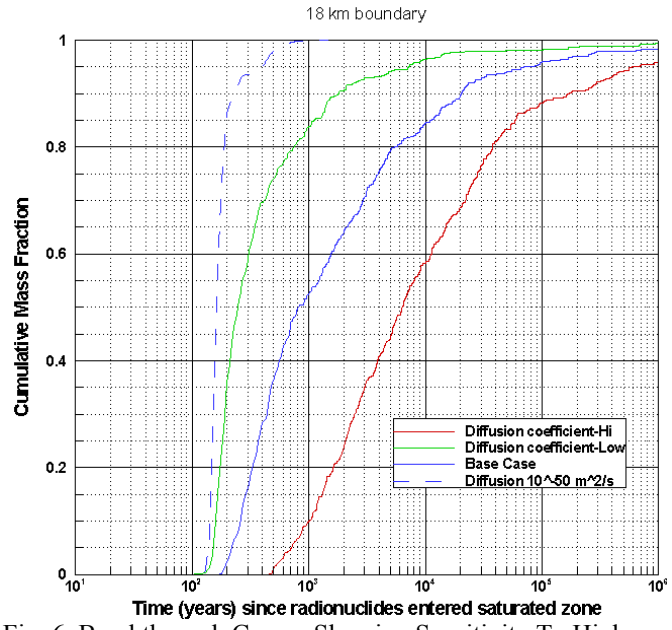

Fig. 6. Breakthrough Curves Showing Sensitivity To High And Low Values Of Diffusion Coefficient.

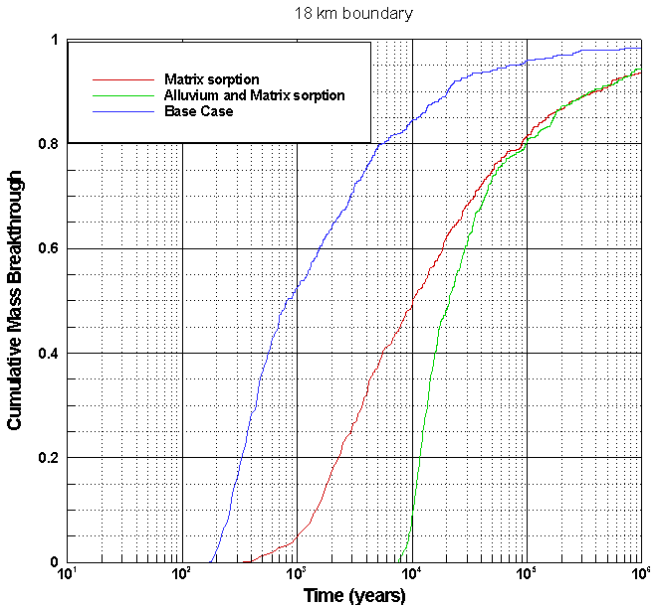

Fig. 7. Effect of sorption on Breakthrough Curves.

A small fraction of colloids with irreversibly attached radionuclides (0.034% to 0.17%, Table 1) has the potential to travel unretarded through the SZ. This fraction has the potential of traveling through within a few tens to a few hundreds of years depending on the value of specific discharge. This fraction is accounted for explicitly in the dose calculations performed for the TSPA. For the largest fraction of the colloids (99.83% or greater), retardation occurs due to the reversible filtration of the colloids themselves in the alluvium and in the fractures within the volcanic units. The radionuclides do not diffuse into the volcanic matrix due to the large size of the colloids. Thus, the matrix diffusion coefficient is set to 0 in this simulation. Figure 8 shows the expected behavior of colloidal-species transport with retardation included in alluvium alone, compared to the base-case aqueous species transport. BT's in the range of 1859 to 688,357 years result for a range of retardation factors of 8 to 5188, indicating significant retardation. Thus, the modeling suggests that for majority of the radionuclide inventory that reaches the saturated zone within the compliance time period, the saturated zone is expected to impart a significant transport time delay.

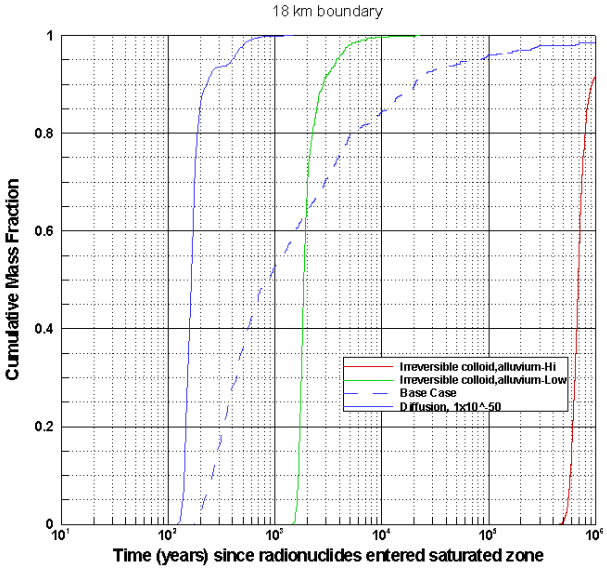

Fig. 8. Comparison of Breakthrough Curves for the Base Case and Radionuclides Irreversibly Attached to Colloids.

The results from simulations that evaluate the effect of changes in distribution parameters for reversible sorption onto colloids in alluvium are shown in Figure 9. For very low values of K_c (10^{-9} m^2/s) the transport is essentially the same as that for base case, and the fastest transport results if the diffusion coefficient in volcanics is also chosen very low, as shown by the solid blue curve giving a BT value around 245 years. The upper limiting value for K_c is of 2×10^3 for americium onto hematite colloids. Using this, the upper limit of the adjusted value of k_d in alluvium becomes 5.0 mL/g. The adjusted minimum effective diffusion coefficient in volcanics of 1.25×10^{-18} m^2/s is used for this case. This is the high curve (labeled "Reversible colloid alluvium-Hi") in Figure 9, giving a BT of 7,023 years, indicating significant delay even for very little matrix diffusion, compared to the base case value of 810 years.

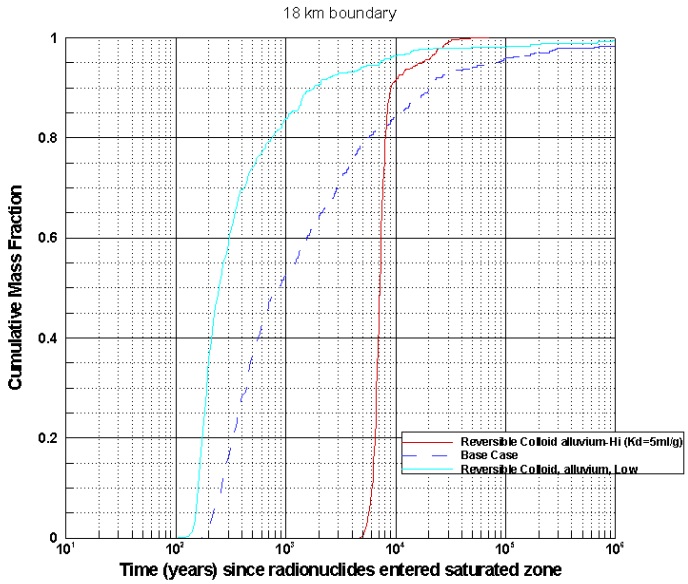

Fig. 9. Propagation of Input Uncertainty in the Colloid Retardation Factor in Alluvium for Reversible Colloids to the Output Breakthrough Curves at the 18-km Boundary.

VI. SUMMARY

A site scale transport model has been developed to simulate the potential transport of radionuclides within the saturated zone at Yucca Mountain for use in the TSPA calculations. It is based on a steady state flow model using the effective continuum approach. The model predicts southerly to south-easterly and sub-horizontal flow near the water table in the vicinity of the Yucca Mountain. The transport model includes the solute transport mechanisms of advection, dispersion, matrix diffusion, retardation due to solute-matrix interactions, and colloid-facilitated transport. The model was validated by comparison with flow paths derived from geochemical data, and by comparing the transit times with those inferred from the ^{14}C data. Uncertainty in the model form is accounted for by considering alternate conceptual models and selecting the base case model that leads to the shortest transit time, i.e. the most conservative model, as well as by modifying the uncertainty distributions of transport parameters.

The base case breakthrough time at the compliance boundary to accessible environment at 18km downstream of the repository for 50% concentration is 810 years. The transport model calculations show that results very with changes in the values of the specific discharge and the matrix diffusion coefficient in volcanic units. Sorption in volcanic rock matrix and in alluvium leads to significant retardation of the sorbing of radionuclides. A small fraction of colloids, explicitly accounted for in TSPA, with irreversibly attached radionuclides (0.17% to 0.034%, Table 1) has the potential to travel unretarded

through the SZ within a few hundreds of years depending on the value of specific discharge. However, for the largest fraction of the colloids (99.83% or greater) with radionuclides attached irreversibly, there is significant retardation, with the range of values of BTs between 4600 to 28519 years. For radionuclides attached reversibly to the colloids, the range of values for BTs is 254 to 7023 years for retardation in alluvium alone, and 165 to greater than a million years for retardation in volcanics alone.

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