From: Paul Bertetti
Sent: Thursday, November 02, 2006 5:08 PM
To: Jude Mcmurry
Subject: FW: TBD No.8 Rev 2
Attachments: DoE_Approach_October_6_2006.ppt

-----Original Message-----
From: hbasagaoglu [mailto:hbasagaoglu@cnwra.swri.edu]
Sent: Friday, October 06, 2006 6:43 PM
To: English Pearcy; David Pickett; Paul Bertetti; Scott Painter
Subject: RE: TBD No.8 Rev 2

Hi All,

I have attached the revised version of it including the saturated zone. More soon,

Have a good weekend,

Hakan

Hearing Identifier: HLW_YuccaMountain_Hold_EX
Email Number: 1076

Mail Envelope Properties (pbertetti@cnwra.swri.edu20061102170800)

Subject: FW: TBD No.8 Rev 2
Sent Date: 11/2/2006 5:08:23 PM
Received Date: 11/2/2006 5:08:00 PM
From: Paul Bertetti

Created By: pbertetti@cnwra.swri.edu

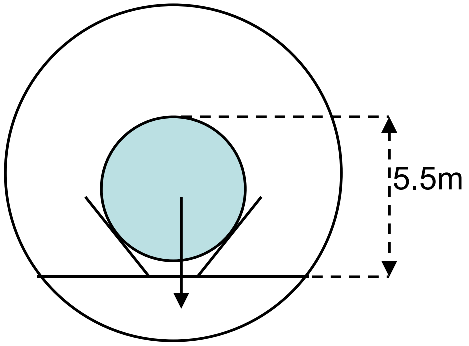
Recipients:
"Jude Mcmurry" <jmcmurry@cnwra.swri.edu>
Tracking Status: None

Post Office:

Files	**Size**	**Date & Time**
MESSAGE	360	11/2/2006 5:08:00 PM
DoE_Approach_October_6_2006.ppt	52801	

Options
Priority: Standard
Return Notification: No
Reply Requested: No
Sensitivity: Normal
Expiration Date:
Recipients Received:

Waste Package (DoE's approach)



Flow domain: In-drift, porous

Potential Colloids to be Generated: smectite (waste glass+clay+mineral), Fe-oxide (corrosion). Humic substances, microbes, and colloids from CSFN, DSFN were excluded. IS determines initial colloid concentrations. The UL of colloid concentration is 200 ppm.

Main Paths: Advection and diffusion (diffusion is Fickian).

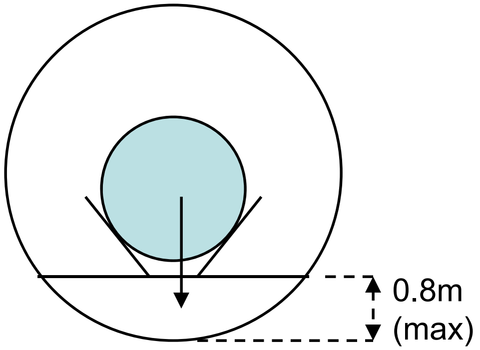
Colloid Stability: Likely to be unstable after post-closure (high evaporation during thermal period, and high IS at later times due to WP failure, leakage, etc.). IS=0.05 is the UL for stability. P_H vs IS determines stability of colloids.
Min colloid concentration is 10^{-6} mg/L (for smectite), 10^{-3} mg/L (for Fe-colloids), when unstable.

Colloid (Physical) Filtration: Potential mechanisms: film and physical straining; surface chemical effect. But, they were excluded in their analyses.

Sorption: 90-99% of Am, Pu irreversibly sorbed only onto Fe-colloids (site-limited, while site-unlimited sorption onto immobile solids). Th, Cs, Pa, St reversibly sorbs onto smectite colloids (and 1-10% Am, Pu reversibly sorbs onto Fe- and smectite colloids. Np and U remains in dissolved phase (low Kd).
Those with Kd>5000 were considered for sorption (piece-wise Kd was assumed). Colloid sorption to air-water interface was excluded (high S_w not expected in WP).

Remarks: Transport Eq., and Kd>5000 is based on constant colloid concentrations.

Invert (DoE's approach)



Flow Domain: Crushed Tuff (with unknown detailed physical specifications)

Potential Colloids to be Generated: Fe-oxide and Cu-oxide, but additional colloid generation is unimportant. **Main Source**: From WP above.

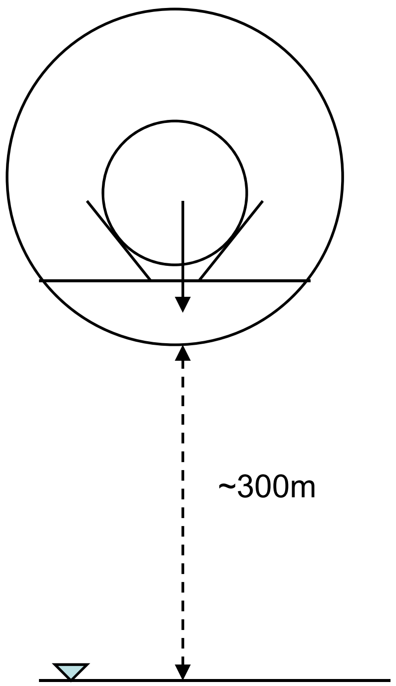
Main Transport Paths: (a) Nominal Case: Intergranular (advection and diffusion in fractures/fissures) – and intraparticle (matrix diffusion). Not significant due to low $D_{colloid}$. (b) Seismic and Igneous scenarios: some advective transport, but depends on stability of colloids.

Colloid Stability: In general, unfavorable (due to high evaporation + high IS). But, to be determined from P_H and IS relations. Matrix pore chemistry determines the colloid stability.

Colloid (Physical) Filtration: Unimportant (due to small filtration depth)

Sorption: No irreversible sorption of radionuclides on colloids (Fe-oxide or Cu-oxide) were allowed. Only reversible sorption of radionuclides onto colloids and immobile phase were considered.

Unsaturated Zone (DoE's approach)



Modeling approach: Very conservative

Flow Domain: TSw (fracture flow with more potentials for physical straining), CH1v (predominantly matrix flow), CH1z (matrix flow) under isothermal condition. Fractured domains presumably consist of well-connected horizontal and vertical fractures.

Potential Colloids (source): Fe-oxide and smectite (size is uncertain)

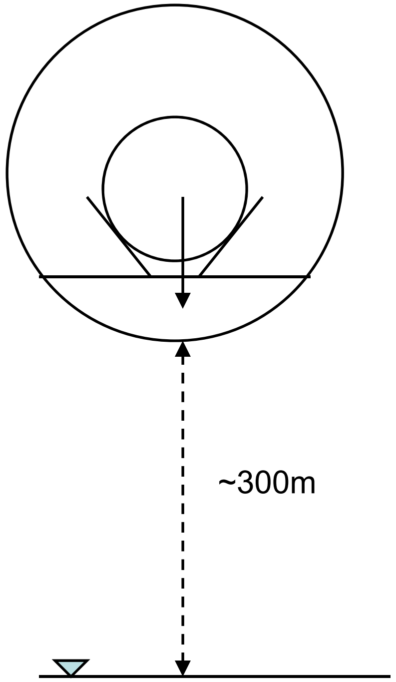
Main Transport Paths: (a) fracture-dominant flow (size exclusion for large particles, physical filtration for small particles; (b) Matrix dominant flow: pore-size exclusion for large particles, surface filtration for smaller particles, and straining filtration (pore size exclusion) for large particle at matrix-fracture interfaces. Advective and dispersive tp in fractures. Diffusion is Fickian.

Colloid Stability: Always stable, unaffected by near field condition (T, geochem, phys)

Colloid Filtration: No sorption and/or filtration of colloids on fracture walls, but only in matrix reversibly or irreversibly (subject to size exclusion a priori).
Film straining (including air-water interface) were excluded. No chemical immobilization.

Sorption: Only 90-99% of Am, Pu can irreversibly sorb onto Fe-colloids, as in WP.
The rest and other radionuclides sorb onto colloids reversibly (the same as in WP).

Unsaturated Zone (DoE's approach)



Main Differences between Process Level Model (PLM) vs. Abstraction Model (AM)

Solution Technique: PLM is a FD model. AM is a particle tracking model.
AM does not suffer from numerical dispersion.

Colloid Diffusion into Matrix: Addressed in PLM, but neglected in AM.

Colloid Tp: Detailed process level simulation in PLM. In AM, colloids are grouped into (a) irreversible fast colloids (no retardation in fractures), and (b) irreversible slow colloids (retardation in fractures). C-Well testing provides the fraction.

Different Processes in Colloidal Tp in UZ than in SZ

- Air-water interfaces, film flow, film straining in UZ.

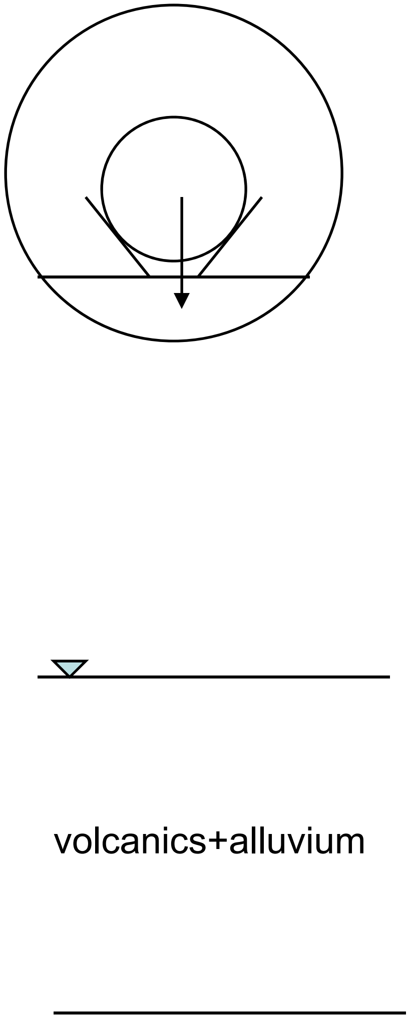
- Slow flow in UZ, which possibly leads to longer reaction times (sorption, etc.).

- More potentials for episodic flows in UZ, which may cause colloid destabilization.

- More potentials for higher IS in UZ, which may affect colloid stabilization.

- Eq. vs non-Eq between matrix and fracture flow and tp in UZ.

Saturated Zone (DoE’s approach)



Modeling approach: No distinction between TSPA and process-level models. Flow was assumed to be steady, and fed into tp model.

Flow Domain: Fractured volcanics (tuffs) and Alluvium

Potential Colloids (source): Fe-oxide and smectite (natural and glass)

Main Transport Paths: By advective water both in tuffs and alluvium.

Colloid Stability: No discussion on this issue.

Colloid Filtration: Filtration rate constant decreases with time (i.e., residence time). A CDF of filtration rate constructed experimentally and used for both alluvium and tuff. Physical straining at the tuffs and alluvium interface. They seem to use the term filtration and sorption interchangably for SZ, may be because they considered matrix diffusion of colloids was negligible in SZ.

Sorption: Mostly first-order rate limited onto fractured walls in volcanics and onto grains in alluvium. A small portion travels unretarded. Pu and Am sorbes onto Fe-colloids irreversibly (90-99%), or embedded in colloids formed from glass products, as in WP and UZ. Matrix diffusion of colloids was negligible (and hence sorption in matrix).

Remarks: Competition between colloids and radionuclides for collector sites was addressed by modified attachments rate of radionuclide as a function of colloid attachment rate (unlike in the other zones). Overall, the retardation in SZ was wiewed as substantial.

Concerns (highlighted by DoE's as well)

Parameters: Used in numerical analyses obtained mostly from lab and/or field tests at scales much smaller than the scale of interest for TSPA.

Validation: Not sufficient field test data for validation of model results.

Uncertainties: Almost in every aspects of their modeling components, seem to be unavoidable.