From: David Brooks
Sent: Thursday, May 17, 2007 2:20 PM
To: James Myers
Cc: James Rubenstone; Randall Fedors
Subject: Fwd:Near Field OR visit
Attachments: UZ-FieldTestTopics_22Mar07 rev1.doc; UZ-FieldTestDocs.doc; 07 3 ENFE TE Agenda1Sep06.doc

Jim - See attached. We need to update and revise the nearfield agenda along the lines of what Randy has produced for the UZ tests. Please take a crack at it and we can refine from that. Also, note (below) email from Debby Barr

email

Dave,

According to the draft meeting list, we're covering the following topics at a meeting on 22-24 May:

Near field environment: Support for modeled evolution of quantity and chemistry of water in the near field, including flux splitting and chemistry deliquescent salts and brines
Multiscale thermohydrologic models: current approach and support for models

Do you think all the right NRC people would be there to include a discussion of the changes in our THC approach? We take a different approach to the starting pore-water chemistry, taking into account characteristics of the current sample set such as completeness and charge balance of the chemical analyses, and indications of sample alteration during sampling and handling. Screened waters were grouped based on numerical evaluation of brine types formed during evaporation, and on multi-variate statistics of variability. We then throw them all in a hat and pull out random samples (just kidding). Actually, the details of the down-selection of the samples are really more than I want to try and cover in an email, and would be better covered in a meeting. The resulting representative set of pore waters are then used as input to a new near-field chemistry (NFC) model we develop in the P&CE to represent seepage water composition in the host rock and the drift environment for use in TSPA. It's based on the IDPS model, with corresponding abstractions for seepage evaporation and invert pore-water composition. The NFC model provides in-drift chemistry and gas compositions, and eliminates the need for chemical binning. These changes also led to the re-evaluation of uncertainties (i.e., the removal of binning uncertainties and inclusion of uncertainties related to the NFC model). The THC model you're familiar with will still be updated and provide the basis for some FEP's exclusions, and may be used as a part of the validation of the NFC model.

We'd like to give you a heads up on this, since you haven't seen it yet, and we thought it might make sense to append it to this meeting. I'm not sure how much we can say about the results, since the P&CE won't be complete until June, but we could at least talk about the development. I don't want to promise too much, since I never know what the current interpretation is on providing preliminary information in meetings. However, I'm hoping we can have a good discussion so you're not taken by surprise later.

>>> James Rubenstone 05/17/2007 7:59 AM >>>
Attached lists developed for the UZ tests Appencix 7, postponed from April.

Hearing Identifier: HLW_YuccaMountain_Hold_EX
Email Number: 486

Mail Envelope Properties (s64c6499.088)

Subject: Fwd:Near Field OR visit
Sent Date: 5/17/2007 2:19:37 PM
Received Date: 5/17/2007 2:20:37 PM
From: David Brooks

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Post Office: NRNWMS05.NRC.GOV

Files	Size	Date & Time
MESSAGE	2875	5/17/2007 2:20:37 PM
UZ-FieldTestTopics_22Mar07 rev1.doc	78401	
UZ-FieldTestDocs.doc	51777	
07 3 ENFE TE Agenda1Sep06.doc	47169	

Options
Priority: Standard
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Sensitivity: Normal
Expiration Date:
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1. Matrix Diffusion

- Describe how the field test information is used in process level and TSPA models
  - Data and interpretations from Alcove 8/Niche 3 (journal articles & AMRs)
    - Are, or will, all available tests and measurements from A8/N3 (Fault Test, Large Plot Test, Tension Infiltrometer, Wetness Sensors) be contained in relevant AMRs? Some questions are:
      - Fault Test: Will effect of ventilation at ESF face outside bulkhead be included?
      - Large Plot: Indications of structural control influencing flow, and alternative conceptualizations (e.g., distribution of seepage flow in subplots, and, flow zones in Salve 2004)
      - Large Plot: Pre-Scrubbing or Post-Scrubbing; specifically, what is the interpretation, and why use one or the other?
      - Tension Infiltrometer bench tests: Do they support fracture hydraulic properties?
      - Large Plot Test: Clarify which geologic properties of the test site (injection unit; TSw33, upper lithophysal), the recovery unit (TSw34, middle non-lithophysal), and the fault that was tested, are most important in interpretation of test results. What geologic evidence supports the application of the test results beyond the test volume and to other faults?
    - How does DOE address the “long-term predictive capability” of the numerical model for sporadic infiltration events with particular reference to their combined numerical and experimental results from Stages 1 and 2 of the most recently reported information on the field experiments?
  - Alcove 6 injection and tracer tests
    - Do the field observations support alternative conceptualizations? (Salve 2002; and Hu et al. 2001, 2002)
  - Alcove 1 infiltration and tracer tests
    - Minimal amount of field data presented
    - Alternative conceptualization: Relationship of MINC parameterization to that of dual-permeability models
  - General questions for field tests and matrix diffusion processes:
    - What is relation between high-flow field tests and low-flow ambient case during postclosure?
    - Explain the basis for the factor of “45” in deriving the empirical diffusion coefficient? What is link between field observations, the factor of “45” for scaling effects.
    - For background, we would like to understand the three factors (and their relative importance) that determine the effective matrix diffusion coefficient: (i) active fracture model parameter, i.e., active fraction of the matrix-fracture interfacial area across which diffusion process takes place, (ii) capillary barrier effects of dry fractures (Seol, Liu, Bodvarsson, 2003, GRL), and (iii) the empirical factor of 45 (that accounts for scaling effects) in determining the effective matrix diffusion coefficient? Which of these three items/parameters dictates the importance of the matrix-diffusion contribution?
    - What is the effect of small-scale fractures in the matrix? Discuss the presence of small fractures noted in observations and their contribution to matrix diffusion.

            - Small fractures may increase the fracture-matrix interface area, and hence increase effective matrix diffusion
            - If intervening large fractures remain “dry,” how do small fractures contribute to matrix diffusion?
            - How is the artificial truncation of fracture abundance data (i.e., >1m length) accounted for in effective matrix area?
            - How does the existence of small-scale fractures affect the ‘importance’ of the matrix diffusion in their conceptual models and how this information was translated into their numerical models?
        - For processes contributing to matrix diffusion, are there field test data support for their relative contributions?
            - Confidence in effective diffusion coefficient values might be improved if field observations can provide insights on each of the contributing processes for matrix diffusion, especially since the tests are done at elevated flux conditions. The different processes lumped into effective matrix diffusion coefficient could be true diffusion, flow into dead-end fractures, alternative fracture pathways, advective flow from fractures into matrix. See also Zhu, Liu, Bodvarsson, and Molz, 2006 paper on “Multi-process matrix diffusion model” that accounts for the effects of (a) stagnant water and infillings, (b) degraded matrix zone, (c) intact matrix zone on the effective matrix diffusion process.
            - The Zhu, Liu, Bodvarsson, and Molz (2006) article, and other articles, appear to represent a different technical basis than in available AMRs – are AMRs being updated to reflect this basis, or does this represent alternative conceptual models?
    - Any other tests supporting a linkage of field data to model support or inputs (including niche dye tracer tests)
- Relationship of active fracture model (AFM) to matrix diffusion results
    - What field observation or additional model support is there for number of flowing fractures, linkage to AFM
    - What field observation or additional model support is there for matrix/fracture surface area (note linkage of AFM coefficient to matrix block size)
    - Contribution of advective flow between fracture and matrix to matrix diffusion
- TSPA--Describe TSPA model results to answer:
    - What fraction remains entirely in fracture throughout UZ?
    - Which rock layer(s) is matrix diffusion a significant contributor as a barrier?
    - What is radionuclide distribution in matrix of each, or selected layers, in the hydrostratigraphic column
    - Possible reasons matrix diffusion being important for UZ, but not for SZ
        - Are the implementations the same?
    - What fractions of matrix diffusion are due to diffusive and advective movement of radionuclides in each hydrostratigraphic unit?
    - When calculating flow fields, is AFM used uniformly for lithophysal and non-lithophysal rocks? for rock with microfractures as well as faults?
    - How can one tell the effect of adsorption in the matrix from that of matrix diffusion with TSPA's results? Any uncertainty/sensitivity analyses to determine the relative importance of each?

2. Seepage (No drift degradation Scenario, Ambient, ~< 50 C)

- Seepage support from small-scale injection tests
  - Anymore Systematic Testing in ECRB? Note, 4 locations total for Tptpll and Tptpmn used in calibration of seepage model
  - Alternative interpretation of tests, successive tests along a borehole
    - Indications that the results reflect characteristics of borehole intersection with fractures of different apertures and orientations
  - Effect of lithophysae or small-scale fractures
    - If quantity of lithophysae might effect seepage, note percentage varies in lithophysal units, and middle nonlithophysal also contains lithophysae
- Seepage support from large-scale injection tests
  - Flow zones: Alternative conceptualization suggested by Alcove 8/Niche 3
  - Structural control: Alternative conceptualization at Alcove 1 and Alcove8/Niche 3 (both fault and large-plot tests)
  - Effects of small faults and fracture zones on seepage distribution across footprint; quantity of faults and fracture zones
  - Are the characteristics of the fractures and faults in the test volumes representative of, or within the range of variability of, those characteristics elsewhere in the repository?
- Are there differences in large-scale and small-scale results, in relation field observations supporting the seepage model?
- Relation of DLS (fracture, fault, and lithophysae) to seepage results
  - Is spacing/quantity of seep points consistent with spacing/quantity of faults, fracture zone, or lithophysal zones (>25% lithophysae)?
  - Is seepage model consistent with intuitive effect of near-horizontal fractures on seepage? Seol et al 2006
- [Lesser Priority] Update on February 2005 seepage event in South Ramp
  - Activities focusing flow patterns on walls and fractures
- [Lesser Priority] Any update on Peña Blanca measurements in and above adits?

3. New Issue, Evaporation from Tiva Canyon

- What field observations support the quantitative estimate of "evaporative concentration" parameter? Were there field observations that prompted DOE to include this new process?
  - Chloride mass balance (CMB) in ECRB, ESF, and surface boreholes based on matrix pore water of varying ages?
  - Temperature profiles from "several" boreholes (out of 18, or 25); Are these consistent with CMB at same locations?
- Can diurnal variations (barometric pumping) or pressure drops from wind-direction based approaches be used to estimate potential evaporative concentration? Are there summer and winter differences? Are there measured flow data from paired boreholes in Tiva Canyon near Highway Ridge Road near crest being used? Where documented? (Ed Weeks in AGU Monograph).
- Are field observations of secondary mineralization consistent with evaporative concentration concept
  - Are there differences between the TCw and TSw? Why expected in one, but not the other?

- CMB requires piston flow and chemical equilibrium between matrix & fracture
  - Are the any observations of fracture water chemistry in UZ?
  - Does perched water reflect chemistry of fracture flow; if so, how does apparent chemical disequilibrium with matrix pore water occur?
- Are there observations or measurement of dried out zones where bedrock is exposed? What is the percent of the area covered by soils?

4. [Lesser Priority] Passive Test in ECRB

- Any updates on data collected and interpretations?
  - In Situ Field Testing Processes AMR
- Are measurements of water potential and saturation in the Passive Test, or ECRB and ESF in general, consistent with surface-borehole data? Only the latter apparently are used for the 3-D UZ mountain-scale UZ flow model calibration.
- How might the results be used to support or modify the seepage model or in-drift convection and condensation model?

5. [Least Priority] Open Technical Agreement, PTn Flow

- Spatial considerations, Lateral flow
  - What are the length scale for lateral flow resulting from Model A and B?
  - What field observations, ESF/ECRB or surface boreholes, were used to support numerical models?
    - DOE notes that heterogeneity can be inferred from 3D calibration (ensemble calibration using the borehole data); i.e., differences between the ensemble calibration the individual boreholes. How does this uncertainty relate to observed heterogeneity in samples from PTn and nature of contacts?
    - Identify the source documents that contains the descriptions of the PTn stratigraphy, and hydrologic and rock properties of the test volume used to support interpretation and extrapolation of the test results
- Temporal dampening of flow
  - Time scale of variation and changes to saturation are important
  - DOE choice for modeling, northern repository thickness not bounding

Recent Journal articles (mostly Alcove 8/Niche 3 & matrix diffusion):

- Hu, Salve, Stringfellow, Wang. 2001. Field tracer transport tests in unsaturated fractured tuff. Journal Contaminant Hydrology 51: 1 –12. [Alcove 6]
- Hu, Kneafsey, Trautz, Wang. 2002. Tracer Penetration into Welded Tuff Matrix from Flowing Fractures. Vadose Zone Journal. Vol. 1. pp. 102–112. 2002. [Alcove 6]
- Liu, Bodvarsson, Zhang. 2004. Scale Dependency of the Effective Matrix Diffusion Coefficient. Vadose Zone Journal 3(1):312-315.
- Liu, Salve, Wang, Bodvarsson, Hudson. 2004. Field investigation into unsaturated flow and transport in a fault: model analyses. Journal of Contaminant Hydrology 74(1-4):39-59.
- Liu, Zhang, Zhou, Molz. 2007. An interpretation of potential scale dependence of the effective matrix diffusion coefficient. Journal of Contaminant Hydrology 90: 41-57
- Salve, Wang, Doughty. 2002. Liquid flow in unsaturated fractured welded tuffs: I. Field Investigations. Journal Hydrology 256: 60– 79.
- Salve, Liu, Cook, Czarnomski, Hu, Hudson. 2004. Unsaturated flow and transport through a fault embedded in fractured welded tuff. Water Resources Research 40, W04210, doi:10.1029/2003WR002571.
- Salve. 2005. Observations of preferential flow during a liquid release experiment in fractured welded tuffs. Water Resources Research 41, W09427, doi:10.1029/2004WR003570.
- Salve and Kneafsey. 2005. Vapor-phase transport in the near-drift environment at Yucca Mountain. Water Resources Research 41, W01012, doi:10.1029/2004WR003373.
- Seol, Liu, Bodvarsson. 2003. Effects of dry fractures on matrix diffusion in unsaturated fractured rocks. Geophysical Research Letters 30(2), 1075, doi:10.1029/2002GL016118.
- Seol, Kneafsey, Ito. 2006. An Evaluation of the Active Fracture Concept in Modeling Unsaturated Flow and Transport in a Fractured Meter-Sized Block of Rock. Vadose Zone Journal 5:1–13.
- Ye, et al. 2007. Assessment of radionuclide transport uncertainty in the unsaturated zone of Yucca Mountain. Advances in Water Resources 30:118-134.
- Zhang, Liu, Zhou, Finsterle. 2006. Effects of diffusive property heterogeneity on effective matrix diffusion coefficient for fractured rock. Water Resources Research 42, W04405, doi:10.1029/2005WR004513.
- Zhou, Liu, Bodvarsson, and Molz. 2006. Evidence of Multi-Process Matrix Diffusion in a Single Fracture from a Field Tracer Test. Transport in Porous Media 63(3): 473-487.
- Zhou, Salve, Liu, Wang, and Hudson. 2006. Analysis of a mesoscale infiltration and water seepage test in unsaturated fractured rock: Spatial variabilities and discrete fracture patterns. Journal of Contaminant Hydrology 87: 96–122.

AMRs:

- Analysis of Alcove 8/Niche 3 Flow and Transport Tests, Rev 00 (2006)
- UZ Flow Models and Submodels, Rev 02 (2004) - ACN 01 (2005)
- Analysis of Hydrologic Properties Data, Rev 00 (2003)
- In Situ Field Testing of Processes, Rev 03 (2004)
- Seepage Calibration Model & Testing Data, Rev 02 (2004)
- Seepage Modeling for PA Including Drift Collapse, Rev 03 (2004)

- Abstraction of Drift Seepage, Rev 01 (2004)
- Conceptual Model and Numerical Approaches for UZ F&T, Rev01 (2004)
- Particle Tracking Model and Abstraction of Transport Processes, Rev 01 (2004)
- Technical Basis Documents for UZ Flow, Seepage, and UZ Transport (2004)

ENFE Technical Exchange Topics
Draft 8/31/06

General

Please include the following information as part of the discussions for each topic area below:

- Any plans for new or revisions to existing abstractions and/or AMRs, including scope and anticipated date(s) for completion/release of the above AMRs; and
- A description of how the information presented during the technical exchange will be incorporated into the TSPA-LA. (Jim, I modified this sentence to emphasize we are staying away from asking DOE to spoon feed us information that is readily available in AMRs, thus our requests for clarification are on aspects that are not clear or that we do not agree --Randy)

B. Seepage flow

1. No drift degradation – Thermally perturbed conditions
    - In-drift convection (based on NRC response to TEF.2.04 and TEF.2.05)
        - Support for FEP'ing out axial redistribution
        - Difference in drift designs used by MSTH and CFD modeling
        - Basis for axial dispersion coefficient applied in MSTH model,
        - Support for CFD model results for redistribution along drifts, particularly when using post-processed CFD air flow results applied to a 1D moisture dispersion model
        - Support for dispersion estimate used in post-processing of CFD model results
    - Thermal Seepage
        - Field observations indicative of preferential flow during thermal tests*
        - Support for results from Birkholzer modification of O.M. Phillips solution, and consistency with abstraction
    - Support for assumption of no gas pressure increase during thermal period, noting the effect of gas pressure on potential brine formation
    - Effect of uncertainties in thermal conductivity of host rock on in-drift temperature and relative humidity, considering
        - In-situ measurements in ESF and ECRB
        - Distribution of lithophysae and other variations in wallrock

2. Degraded drift –Ambient conditions
    - Incorporation of seepage (dripping and along-wall flow) at degraded ceiling
    - Clarification of water flow through rubble
        - Characterization of rubble and relevant flow processes
        - Hydrologic effect of fine particles settling to lower part of rubble pile in contact with DS, or, if DS degraded, with WP

3. Degraded drift – Thermally perturbed conditions
    - Heat transfer (convection, radiation, and conduction) through rubble
        - Estimation of effective thermal conductivity in rubble
        - Effect of high gradient in temperature in lower portion of rubble near DS or WP on vaporization barrier and salt precipitation
    - Thermal seepage in rubble

* possible OR topic

        - Support for vapor barrier effectiveness in rubble when modeled as homogeneous dual permeability media with REV potentially larger than grid scale
    - In-drift convection in partially degraded drift considering:
        - Intact DS and possibility of significant air gap above rubble
        - Convection between sections of degraded drift (e.g., scale of several WP)

4. Discussion of natural ventilation exchange with the atmosphere*
    - Will exchange of air through closed (partially blocked) ventilation shafts that may reduce relative humidity in the drifts be included in LA?
    - Update on understanding of other processes that might affect relative humidity in drifts (S&T work)

C. Flux splitting
- Discussion of flow through stress corrosion cracks for the drip shield and waste package including:
    - Theoretical approach and bases
    - Planned experiments
    - Recent experimental results
- Discussion of flux splitting in intact and degraded drift scenarios including
    - Mass balance of moisture (seepage and condensation) into and/or through (integration between natural and engineered systems):
        - drip shield;
        - waste package; and
        - invert
        - UZ below invert
    - Clarification of how porous media model incorporates flow along drift walls
    - Role of dripping from drift walls and rock bolts when not above drip shield
    - Role of film/rivulet flow. If it is not considered, why? (Pavan, please clarify what you are getting at here, film and rivulet flow where? –Randy)

D. Deliquescence Chemistry
- Detailed discussion of the bases for screening out localized corrosion due to salt deliquescence
- Detailed discussion of recent atmospheric dust sampling and analyses* including:
    - Planned or completed sampling events including locations and analyses
    - Results of sample analyses including samples collected at the south portal and any other dust analyses not available to the public.
    - Availability and quantity of split samples

E. Seepage chemistry
- Detailed discussion of the seepage water chemistry binning process including
    - THC modeling input parameters and intermediate outputs*
    - Locations of nodes sampled from TOUGHREACT modeling outputs*
    - Temperatures that waters were evaporated to activity of water = 0.65*
- Discussion of the results of THC modeling for the degraded drift scenario
    - Concentrations nitrate and other inhibitor species

* possible OR topic

    - Ratios of Chloride to inhibitor species concentrations
- Discussion of any planned changes to the binning approach used in the seepage water chemistry abstraction and TSPA-LA.

F. Post-Heater Test Results
- Discussion of sampling and analyses
    - Locations and types of samples collected or planned for collection
    - Types of sample analyses completed or planned
    - Results of sample analyses including
        - Chemistry of dust*;
        - Chemistry of corrosion products/residues*; and
        - Analyses of rubble due thermal spalling including quantity and size distribution*

- How are the post-heater test results going to be incorporated in the near field model abstractions and AMRs?

G. Open KTI agreement items

* possible OR topic