UNITED STATES
NUCLEAR REGULATORY COMMISSION
WASHINGTON, D.C. 20555-0001

January 26, 2001

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Office of Licensing and Regulatory Compliance
U.S. Department of Energy
Office of Civilian Radioactive Waste Management
Yucca Mountain Site Characterization Office
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SUBJECT: U.S. NUCLEAR REGULATORY COMMISSION/U.S. DEPARTMENT OF ENERGY TECHNICAL EXCHANGE AND MANAGEMENT MEETING ON EVOLUTION OF THE NEAR-FIELD ENVIRONMENT (JANUARY 9 - 12, 2001)

Dear Mr. Brocoum:

Enclosed are the meeting summary highlights agreed upon during the January 9 - 12, 2001, Technical Exchange and Management meeting between the staff of the U.S. Nuclear Regulatory Commission and the U.S. Department of Energy. The main purpose of the meeting was to discuss one of the Key Technical Issues, Evolution of the Near-Field Environment (ENFE). The meeting was held in Pleasanton, California.

If you have any questions regarding this letter, please contact the technical lead for ENFE, Mr. Bret Leslie or the Senior Project Manager for issue closure, Mr. James Andersen. Mr. Leslie can be reached at (301) 415-6652 and Mr. Andersen at (301) 415-5717.

Sincerely,

C. William Reamer, Chief
High-Level Waste Branch
Division of Waste Management
Office of Nuclear Material Safety
and Safeguards

Enclosure: Summary Highlights of NRC/DOE Technical Exchange and Management Meeting on Evolution of the Near-Field Environment

cc: See attached distribution list

Letter to S. Brocoum from C.W. Reamer dated: January 26, 2001

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Summary Highlights of NRC/DOE Technical Exchange and Management Meeting on Evolution of the Near-Field Environment

January 9-11, 2001
Pleasanton, California

Introduction and Objectives

This Technical Exchange and Management Meeting on the Evolution of the Near-Field Environment (ENFE) is one in a series of meetings related to the U.S. Nuclear Regulatory Commission (NRC) key technical issue (KTI) and sufficiency review and the U.S. Department of Energy (DOE) site recommendation decision. Consistent with NRC regulations on prelicensing consultations and a 1992 agreement with DOE, staff-level resolution can be achieved during prelicensing consultation. The purpose of issue resolution is to assure that sufficient information is available on an issue to enable the NRC to docket a proposed license application. Resolution at the staff level does not preclude an issue being raised and considered during the licensing proceedings, nor does it prejudge what the NRC staff evaluation of that issue will be after its licensing review. Issue resolution at the staff level, during prelicensing, is achieved when the staff has no further questions or comments at a point in time regarding how the DOE is addressing an issue. The discussions recorded here reflect NRC's current understanding of aspects of the ENFE KTI most important to repository performance. This understanding is based on all information available to date which includes limited, focused, risk-informed reviews of selected portions of recently provided DOE documents (e.g., Analysis and Model Reports (AMRs) and Process Model Reports (PMRs)). Pertinent additional information (e.g., change in design parameters) could raise new questions or comments regarding a previously resolved issue.

Issues are "closed" if the DOE approach and available information acceptably address staff questions such that no information beyond what is currently available will likely be required for regulatory decision making at the time of any initial license application. Issues are "closed-pending" if the NRC staff has confidence that the DOE proposed approach, together with the DOE agreement to provide the NRC with additional information (through specified testing, analysis, etc.) acceptably addresses the NRC's questions such that no information beyond that provided, or agreed to, will likely be required at time of initial license application. Issues are "open" if the NRC has identified questions regarding the DOE approach or information, and the DOE has not yet acceptably addressed the questions or agreed to provide the necessary additional information in a potential license application.

The objective of this meeting is to discuss and review the progress on resolving the ENFE KTI (see Attachment 1 for the description of Subissues #1, 2, 3, and 4). Subissue #5, "Effects of Coupled Thermal-Hydrologic-Chemical Processes on Potential Nuclear Criticality in the Near Field," was discussed during a Technical Exchange and Management Meeting on October 22-23, 2000, and was not discussed during this meeting. The quality assurance (QA) aspect of this KTI was determined to be outside the scope of the meeting and is being tracked in NRC's ongoing review of DOE's QA program.

Summary of Meeting

At the close of the Technical Exchange and Management Meeting, the NRC staff stated that Subissues 1, 2, 3, and 4 were "closed-pending." Specific NRC/DOE agreements made at the meeting are provided as Attachment 1. The agenda and the attendance list are provided as Attachments 2 and 3, respectively. Copies of the presenters' slides are provided as Attachment 4. Highlights from the Technical Exchange and Management Meeting are listed below.

Highlights

1) Opening Comments

DOE stated that the intent of the meeting is to reach agreement on the current status and path forward for each of the ENFE subissues (see "Evolution of the Near Field Environment" presentation given by Deborah Barr). In the ENFE Issue Resolution Status Report (IRSR), Revision 3, the NRC stated that ENFE Subissues 1, 2, 3, and 4 are "open." During this meeting, DOE stated that its presentation would focus on confirmatory and additional information, data, and analyses identified by the NRC in the IRSR and subsequent discussions. DOE stated that it felt that the details provided during the current meeting would be the basis for NRC to list Subissues 1, 2, 3, and 4 as "closed-pending." The DOE presented several viewgraphs which provided a road map identifying which DOE presentations address each NRC comment. The NRC inquired about two of the items listed. First, the NRC staff asked when the TOUGHREACT executable will be available; the DOE stated it would provide that information at a later time (see Agreement 1 of Subissue 4). Second, the NRC asked for some discussion during this meeting of retardation and matrix diffusion parameters under thermal-hydrologic-chemical (THC) conditions.

2) Total System Performance Assessment

NRC Comments Related to TSPA Treatment of Engineered Barrier System Chemical Environments

The DOE gave an overview of the TSPA model treatment of the engineered barrier system (EBS) chemical environment, with reference to NRC comments from Revision 3 of the ENFE IRSR and subsequent telephone discussions emphasizing how couplings are taken into account. Seepage water and gas compositions are calculated using the drift-scale THC seepage model for four periods during repository thermal evolution. The NRC expressed particular interest in how parameter uncertainties are propagated through the models. The DOE responded by addressing hydrologic parameter uncertainties and conceptual model uncertainties and indicated their belief that uncertainty propagation would have insignificant effects on model results. The NRC stated that it was not convinced that uncertainty propagation will have insignificant effects on model results. The DOE stated that this issue will be touched on in subsequent presentations. The presentation then addressed a comment from ENFE IRSR, Rev. 3 concerning the lack of coupling among several process models involving the chemical environment. The DOE responded by describing integration of many models, such as gas flux/composition and precipitates/salts, with THC abstractions. The DOE considers that model integration/coupling will be sufficient for describing the model EBS chemical environment, taking into account completed and ongoing work. The NRC asked for the

technical basis supporting the DOE conclusion that interactions between water and engineered materials would have negligible impact on performance. The DOE referred to a general discussion in the corrosion AMR and mentioned modeling results on steel corrosion product effects. The NRC stated that this argument needed to be strengthened. In response to an NRC question on the range of gas fluxes modeled, the DOE referred to the EBS Physical Chemical Environment AMR. The NRC also asked why nitrate was not included among modeled species. The DOE answered that its corrosion modelers did not consider nitrate to play an important role. In response to another NRC question, the DOE stated that, currently, they did not believe propagation of uncertainty among coupled process models would significantly change the results. The NRC stated that the DOE needed to provide additional technical bases that this approach is adequate.

The DOE then addressed two comments from Revision 3 of the ENFE IRSR on in-drift colloid transport modeling. The in-drift water chemistry model treatment was argued to be conservative, as was the exclusion of alternative conceptual transport models. The NRC asked if the DOE considered colloid entrainment by vigorous water movement in the drift. The DOE answered that they had not considered this but would expect the effect on transport to be small due to (1) low flow rates in the drift and (2) the tendency of boiling-generated flow to be directed toward the source.

NRC Comments Related to TSPA for the Site Recommendation Results Related to Waste Form Degradation

This presentation focused on the TSPA-SR waste form degradation model. The in-package chemistry and colloid concentration components were addressed to answer the NRC comments under Subissue 3. The DOE stated that this presentation provided context for more detailed discussions to be presented in subsequent talks and provided the basis for resolution of five NRC Subissue 3 comments. The in-package chemistry component - new to TSPA - is directly coupled to model components covering waste degradation and radionuclide concentration. Included chemical parameters are pH, ionic strength, and chloride. Bulk chemistry calculations, at the package scale, are used so that localized effects such as radiolysis are not included, but have been evaluated. Next, the colloid release model component was described. The model includes reversible and irreversible attachment, assumes no filtration or sorption of colloids within the package, and incorporates pH and ionic strength effects. The DOE has concluded that colloids are minor contributors to dose. The DOE then addressed three comments from Revision 3 of the ENFE IRSR regarding colloid release. The first comment concerned the current exclusion of release of waste-form colloids from spent nuclear fuel. The DOE will continue to monitor drip corrosion tests for possible colloid production. The second NRC comment related to neglecting of chemical effects other than pH and ionic strength effects. The DOE indicated that they will in future reports strengthen arguments supporting the neglect of chemical effects. The third NRC comment related to the selection of radionuclides included in colloid modeling. The DOE made qualitative arguments for the selection of radionuclides included in colloid modeling. The NRC raised a number of questions concerning colloid modeling. The NRC stated that it was looking for a more quantitative basis for the radionuclide selection. In its response, the DOE reiterated the dose-effect basis it had presented. Two questions concerned the impact of the ionic strength stability effect on radionuclide mobility. The DOE stated that in its models, colloids were consistently at their maximum stability levels, so that the highest possible colloid concentrations are being modeled. The NRC pointed out

that it may be inappropriate to evaluate the proportional dose importance of colloids by comparison to aqueous release, which may be much less mobile than colloid releases. The NRC asked if model results on relative concentrations of aqueous and colloidal plutonium release have been compared directly to Argonne National Laboratory test results. The DOE said that they had not made this comparison. The NRC commented that it would be informative to show how the quantity of colloids produced compared to the in-package chemistry-limited-values, released from the waste package to the invert. The NRC asked whether it was possible that the dose-based radionuclide selection process could be circular. The DOE answered that their selection process, while qualitative, was initiated in the absence of any dose contribution information. The NRC suggested that this process is not well documented. Finally, Mr. Don Shettel (Nye County) asked why the DOE had not used vadose zone water equilibrated with tuff for corrosion tests. The DOE stated that the in-package concentration are not sensitive to the range of influent water compositions used.

The NRC inquired about the method used to solve for pH in the "in-package chemistry model." For example, pH is used in the calculation of the rate of high-level waste dissolution and the rate of high-level waste dissolution is a function of pH. The DOE stated that the pH is calculated in a step-wise (temporally) manner.

TSPA Representation of Effects of Coupled THC Processes on Radionuclide Transport

The DOE discussed the incorporation of THC effects in the EBS transport abstraction in TSPA. Currently, the DOE takes no credit for retardation within the EBS. The NRC had provided comments to the DOE on this topic under Subissue 4. These comments had been resolved prior to the meeting. This abstraction integrates information on seepage and flow, thermal evolution, waste package corrosion, and water compositions as affected by EBS materials. Diffusive transport is modeled to begin as soon as stress corrosion cracking affects the waste package, irrespective of drip shield failure. Advective release requires formation of waste package general corrosion patches. In response to the NRC questions, the DOE said that: (1) they may in the future include EBS radionuclide retardation in the invert and on corrosion products as part of efforts to reduce conservatism; and (2) they have done calculations showing that the waste package flow-through model approach is conservative.

The NRC questioned whether the flow-through model was most conservative with respect to peak mean dose. In particular the NRC submitted that a "draining bath-tub" would release mass more quickly. However, the NRC submitted that the risk significance of this alternative release model was not known. The DOE stated that their selection of the EBS release model was conservative with respect to earliest release.

3) Technical Discussions - Subissue #1, Effects of Coupled Thermal-Hydrologic-Chemical Processes on Seepage and Flow

NRC Comments on Coupled Thermal-Hydrological-Chemical Processes Affecting the Calico Hills Hydrogeological Unit Related to Subissue 1

A summary of the current status of resolution was presented (see "NRC Comments on Coupled Thermal-Hydrological-Chemical Processes Affecting the Calico Hills Hydrogeological Unit Related to Subissue 1" presentation given by Eric Sonnenthal). This presentation addressed

comments from Revision 3 of the ENFE IRSR that indicated that the DOE needs to evaluate the potential effects on performance (e.g., shorter travel time, diminished sorption) of alteration of the Calico Hills nonwelded unit (CHn) below the repository. The DOE has concluded that any changes to CHn resulting from the excursion up to approximately 75°C will have negligible impact. The key line of reasoning is that alteration of clinoptilolite to analcime will be kinetically and thermodynamically inhibited due to the abundance of silica. Furthermore, the DOE has concluded that any alteration of zeolite properties (in the absence of alteration to analcime) would be minor. These conclusions may be tested in the future by mountain-scale THC models. In response to an NRC question, the DOE stated that it has not yet decided whether this modeling will be performed. The NRC asked if the DOE had considered the alteration of glass to zeolite. The DOE said this minor effect had been discussed in the AMR on drift-scale coupled processes. This AMR is also the source of validation information requested in another NRC question. The NRC asked if there was a threshold temperature at which the mineral transformation will be important. The DOE answered that the temperature is dependent on particular conditions and that, in any case, it is above 70°C for CHn alteration. The NRC asked if advective removal of silica was considered because slow silica removal is central to their argument. The DOE considered the different flow regimes (in vitric and zeolitic minerals) present in the CHn. The DOE stated their model considered inter-fingering of vitric and zeolite minerals and should bound possible flow regimes. The NRC asked about uncertainty propagation in the handoff of drift-scale THC calculations to other abstractions. The DOE stated that it considered the use of the two mineral models (simple and complex) and the representation of infiltration uncertainty to bound uncertainties. The NRC acknowledges that the performance impact of CHn alteration is minor under the current DOE model approach in which only a portion of unsaturated zone flow from the repository traverses the CHn. Performance impact will need to be reassessed if that assumption changes.

Subissue 1: NRC Comments on Thermal Alteration of the Paintbrush Tuff Nonwelded Hydrogeological Unit

A summary of the current status of resolution was presented (see "Subissue 1: NRC Comments on Thermal Alteration of the Paintbrush Tuff Nonwelded Hydrogeological Unit" presentation given by Nicolas Spycher). In this presentation, the DOE addressed the NRC comments regarding the DOE neglect of repository-driven alteration of the Paintbrush Tuff Nonwelded (PTn) unit above the emplacement zone. The DOE has determined that effects of alteration of the PTn on performance would be negligible. The THC modeling indicates that permeability and porosity changes would be negligible. The PTn is modeled to be above 40°C for about 2000 years and predicted porosity decreases are less than 0.005 percent. Results of this modeling and sensitivity studies are to be documented in future DOE reports and work is still in progress.

Subissue 1: Comments on Effects of Cementitious Materials

A summary of the current status of resolution was presented (see "Subissue 1: Comments on Effects of Cementitious Materials" presentation given by Ernest Hardin). This presentation was focused on addressing a comment from Revision 3 of the ENFE IRSR on the need for the DOE to analyze and evaluate the potential for interaction between cementitious materials and host rock that may affect flow and transport. The DOE stated that analyses of the effects of cement grout for rockbolts are reported in the EBS Physical and Chemical Environment AMR Rev 01.

The DOE stated that these analyses concluded that effects on gas and water compositions will be minor. Grout leachates will comprise only a few percent of the total seepage into the drift. The DOE described proposed additional mountain-scale THC modeling expected to further support their exclusion of cement influence. Key mitigating processes include leachate dilution, leachate neutralization by gas-phase carbon dioxide, and permeability reduction by calcite precipitation. The DOE stated that information in planned updates to AMRs and PMRs will bolster their argument. The NRC asked whether the DOE believed they could further support the exclusion without new modeling. The DOE responded that mass balance considerations may be sufficient. In response to a question from Mr. Carl DiBella (Nuclear Waste Technical Review Board - NWTRB staff), the DOE said that discussion of a relevant anthropogenic analog is included in the EBS Physical and Chemical Environment AMR Rev 01.

Subissue 1: NRC Comments on Mineral Precipitation in Fractures or at the Fracture-Matrix Interface

A summary of the current status of resolution was presented (see "Subissue 1: NRC Comments on Mineral Precipitation in Fractures or at the Fracture-Matrix Interface" presentation given by Eric Sonnenthal). This presentation addressed the NRC comments on modeling approaches related to THC processes including fluid dynamics at the boiling front and the treatment of dry fracture blocks. The DOE has determined that effects of mineral precipitation on hydrologic properties can be neglected based on modeling which shows that fracture sealing will not occur. The DOE asserted that these conclusions are supported by Drift Scale Test results. The NRC asked, considering the three year duration of the drift scale test, how can one conclude that there is no bulk fracture sealing. An example was given that if the rate of deposition was one percent per year, only three percent of the fracture porosity will have sealed over the test duration which is likely to not be observable with current measurement techniques. The DOE stated that the observations to date provide constraints to some of the reaction rates. Model assumptions regarding the boiling front are justified by sensitivity studies and the modeled demonstration of conservation of mass. Results are stated to be in the Unsaturated Zone Flow and Transport milestones which the NRC requested the DOE to provide. Discussion of numerical modeling of the dry-out front and reactive surface areas prompted a request from NRC for information on the modeled quantity of unreacted solute trapped in a non-physical manner produced in the dry-out zone. The NRC also requested information on available physical evidence from the Drift Scale Test which would support the DOE's precipitation model predictions. The NRC inquired as to the validity of the active fracture model during the thermally-perturbed time period. The DOE responded that this point should be evaluated but that they believe water flow is appropriately represented during ambient and thermally perturbed conditions.

The NRC expressed the concern that the various sources of uncertainty, such as data uncertainty, conceptual model uncertainty, and model implementation result in very uncertain output. The NRC inquired whether the DOE's treatment of uncertainty in the drift-scale THC model appropriately represented and propagated uncertainty from the various sources. The DOE agreed that the uncertainties are large and felt that comparison to experimental results are the way to build confidence in the model results. The DOE stated that some sealing does occur in small fractures, based on laboratory experiments. The NRC questioned what implications to the seepage or radionuclide transport models may be if sealing of small

fractures occurred but bulk permeability was minimally reduced. The DOE stated it would most likely depend on how the final distribution ended up.

During the public comment section, Mr. Steve Frishman (State of Nevada) asked what is the fate of the mobilized silica and how is it treated in terms of conceptual models.

ENFE Subissue 1 Overall Status

As a result of additional discussions, the NRC and DOE reached seven agreements for Subissue #1 (see Attachment 1). With these seven agreements, the NRC stated that Subissue #1 could be listed as "closed-pending".

4) Technical Discussions - Subissue #4, Effects of Coupled Thermal-Hydrologic-Chemical Processes on Radionuclide Transport

Subissue 4: NRC Comments on Colloidal Transport in the Unsaturated Zone

A summary of the current status of resolution was presented (see "Subissue 4: NRC Comments on Colloidal Transport in the Unsaturated Zone" presentation given by Jim Houseworth). The DOE addressed a comment from Revision 3 of the ENFE IRSR that the DOE provide additional technical bases supporting models and data for simulating unsaturated zone colloidal transport. The DOE described the colloidal transport model, noting conservatisms such as neglect of colloid diffusion, confining most colloids to fracture transport, and neglect of colloid retardation. The presentation included a description of how the distribution for the colloidal radionuclide transport parameter K_c was determined using the maximum model colloid concentration determined using an empirical relationship to ionic strength, and the high K_d for Am on smectite. The NRC asked if the DOE had screened out THC effects on transport parameters such as sorption coefficient and aqueous speciation. The DOE responded that THC screening was in reference to effects on rock properties, and that chemical effects on transport-relevant properties (including colloids) had not been explicitly addressed. The DOE stated that the broad distribution range for K_c may encompass all possible effects. The NRC suggested that waters collected during the drift-scale test (none have yet been observed) may yield colloid information, and that ongoing studies at Rainier Mesa may also be pertinent. The DOE answered that they will look at such data, but that they are unlikely to add information because the DOE is assuming no colloid retardation. The NRC asked if the maximum colloid concentration used in calculating K_c is bounding with respect to perturbed conditions; the DOE answered that this value reflects ionic strength relationships under ambient conditions. Finally, the NRC asked whether the DOE had considered possible entrainment of colloids and particulates in convecting/advecting fluids during boiling. The DOE said that they had not, but that low fluid fluxes made it unlikely that this effect would be significant.

As a result of additional discussions, the NRC and DOE reached eight agreements for Subissue #4 (see Attachment 1). With these eight agreements, the NRC stated that Subissue #4 could be listed as "closed-pending".

5) Technical Discussion - Subissue #2, Effects of Coupled Thermal-Hydrologic-Chemical Processes on the Waste Package Environment

The NRC staff made available their concern on the technical basis for treatment of FEP 1.2.06.00 (Hydrothermal activity) they had presented verbally on January 8, 2001, during the Thermal Effects of Flow (TEF) Key Technical Issue Technical Exchange (see Attachment 4, Presenter's Slides).

Subissue 2: NRC Comments on In-drift Geochemical Environment

A summary of the current status of resolution was provided in the first DOE presentation (see "Subissue 2: NRC Comments on In-drift Geochemical Environment", presentation given by Ernest Hardin). The purpose of the presentation was to address the NRC concern that the incomplete description of the geochemical environment, including introduced materials and trace elements, does not allow the DOE to calculate or bound, using local reactions and reaction paths, the potential geochemical environments that may be important to the performance of the drip shield and waste package. Additionally, the presentation addressed the NRC's concern on the DOE's approach to complete a final design that accounts for: (a) impacts of in-drift materials on the geochemical environment and repository performance; and (b) definition of those materials that could be incorporated into the emplacement area.

The DOE's basis for resolution includes their technical judgement that the current models produce expected and bounding compositions based on the behavior of major and minor chemical species. The DOE's approach currently uses bulk chemical calculations. The NRC staff questioned the importance of local reactions on the variability and uncertainty of downstream performance assessment models. The DOE responded that heterogeneities are not important from a features, events, and processes screening approach. Responding to an NRC question, the DOE indicated that fluoride could be calculated in the process-level models, but it is not used in total system performance assessment models. The NRC staff expressed a concern that the current DOE approach does not bound the possible water chemistries, rather it provides boundary conditions to the exisiting models. For instance, the NRC indicated that the current two conceptual models used to calculate the composition at the drift wall are not necessarily bounding. The NRC also inquired as to how the waters could be considered bounding considering the impact of the degradation of introduced materials. The DOE presented, in tabular form, a comparison of various waters. In particular water predicted for seepage period 2 at a relative humidity of 95%, cement leachate, and equilibriated leachate were compared. The DOE stated that the compositions of these waters were similar. The NRC pointed out that aluminum was quite a bit (three orders of magnitude) higher in the cement-reacted waters than the other waters. In addition, the NRC commented that they expected the evaporation of the cement leachate waters may result in compositions that are significantly more concentrated in some species than the evaporated seepage water. As an additional basis, the DOE indicated that planned activities to evaluate alternative reactions and reaction paths would be documented in updates to the engineered barrier system geochemical models. The activities would focus on trace elements (lead, mercury, and arsenic, and expanded as necessary) that have been suggested to be important to the performance of the EBS. A further basis for resolution is additional work being performed on revising the Pitzer database, and work that is being considered to modify the EQ3/6 computer code. The DOE indicated that the current baseline control process (AP-3.4Q) is a basis to resolve the NRC's concern on the DOE's approach to a final design.

The NRC staff stated that the planned activities do not clearly address their concerns on the materials, their compositions and reactions, and their potential importance to repository performance. The DOE's response was two-fold. First, the DOE indicated that efforts to characterize trace elements in the natural environment, in rocks and fluids, can be completed and efforts are ongoing. Regarding the focus of the NRC's concern, the DOE indicated that they would evaluate trace elements in steel and concrete. Once the inventory activity was completed, they would model the environment focusing on lead, mercury, and arsenic.

Mr. Don Shettel (Nye County) asked DOE which trace elements were important to the drip shield performance. The DOE responded that the review process is still underway and the list has not been finalized. The NRC staff asked whether there are plans for additional uncertainty analyses for reaction pathways. The DOE responded that they had not yet closely looked at reaction pathway uncertainties.

Evolution of the Near-Field Environment Subissue 2: NRC Comments on Treatment of Coupled Process and Model Integration

The second DOE presentation (see "Evolution of the Near-Field Environment Subissue 2: NRC Comments on Treatment of Coupled Process and Model Integration" presentation given by Ernest Hardin) addressed two NRC concerns. The first NRC concern is that there is an inadequate technical basis to support DOE's approach that coupled THC processes can be decoupled, evaluated separately, and then re-coupled, without adversely affecting predictions of repository performance. The second NRC concern is that the DOE's Physical and Chemical Environment sub-models are insufficiently integrated and that the use of J-13 water composition as an initial condition is inappropriate. The DOE addressed these concerns using three discussions. The first discussion focused on coupling relationships and also addressed an alternative approach that is being considered. The second discussion on mass and energy fluxes addressed the technical basis for separating sub-models. The final discussion on model integration addressed the concerns on insufficient integration and the use of J-13 water composition.

In the first discussion the DOE indicated that the basis for resolution is that thermal-hydrological coupling effects are already included, thermal effects on chemistry have been addressed, and that small-scale coupling relationships are addressed empirically. The DOE indicated that another basis for resolution is that other in-drift thermal-hydrological-chemical processes are negligible. The NRC questioned whether these arguments had been documented and the DOE stated that specific in-drift coupling relationships have been and will be addressed in a variety of revised reports. The DOE added that the drift-scale test represents the coupled processes pertinent to Yucca Mountain. For example, electrical potential variations have been observed in the rock near the wing heaters. The NRC asked what was the magnitude of the electrical potential variation. The DOE responded it was several hundred millivolts. The NRC staff asked whether the potential for rockfall on the drip shield denting the shield and subsequent impacts of fluid collection in the dent had been evaluated. The DOE indicated that this has been addressed in the stress corrosion cracking analysis/model report. The NRC questioned what changes were documented concerning microbial processes and whether the model had been supported by data. The DOE indicated that production of carbon dioxide and the presence of a localized biofilm had been addressed and the validation information was included in the revised microbes report. The DOE outlined an alternative proposed approach that would include the in-

drift environment on the same thermal-hydrological-chemical simulations that are now used for the host rock. The NRC questioned at which locations the model would be applied. The DOE indicated that the main focus would be application in evaluating changes to the diffusivity properties of the drift invert. The NRC asked what the importance of the porosity of the deposited minerals/salts would be with respect to the deliquesence point. The DOE responded that observations from mechanical engineering, when determining the deliquesence point of salts, suggest the effect to be of minor importance.

The second discussion focused on mass and energy fluxes. The DOE asserted that processes can be separated, simulated, and re-coupled provided that important interactions are included. The NRC stated that this conclusion is conditional on the assumption that various sources of uncertainty from sub-models are propagated through the analysis. The DOE stated that the impact of various sub-models on the physical and chemical environment is documented in a variety of revised reports. The primary basis for DOE assertions that models can be simulated separately is that interactions between locations are unimportant if there is no solid or liquid mass transfer. Because gravity is the dominant physical process controlling liquid transfer, only those models directly tied via liquid flow pathways are coupled. All models that are dependent on oxygen and carbon dioxide concentrations are coupled to the processes affecting gas composition. The DOE indicated that they are investigating small-scale interactions in the materials testing program. The NRC questioned the technical basis for the DOE screening out the effects of fluids interacting with grouted rock bolts. The NRC asked whether the DOE has adequately addressed the chemistry of initial fluids formed upon re-wetting of evaporated salts. The DOE stated that separation of physical and chemical process submodels is justified by the separation of key locations within the EBS. Interactions between locations would be unimportant if there is no solid or liquid mass transfer. The NRC commented that it is difficult to determine when interactions between locations are unimportant because the chemical divide process in an evaporative system can result in small uncertainties being propagated into large effects.

The final discussion on model integration offered two bases for resolution. First, the DOE indicated that current models use abstracted water compositions from thermal-hydrological-chemical modeling of the host rock as the drift-wall boundary conditions. Second, the DOE indicated that the type of water represented by thermal-hydrological-chemical model results (chloride-sulfate type) has been incorporated in corrosion testing.

Subissue 2, NRC Comments on the Assumption of Chemical Equilibrium

The third DOE presentation (see "Subissue 2, NRC Comments on the Assumption of Chemical Equilibrium" presentation given by Ernest Hardin) addressed the assumption of equilibrium in chemical models in the salts/precipitates analyses in response to an NRC comment requesting a stronger technical basis for this assumption. The response focused on similarities between laboratory and model results. In addition, suppressed minerals in models were selected based on known paragenesis, and suppressions and alternate precipitates are tested in sensitivity studies. The NRC questioned the extent of the technical basis used in determining mineral suppressions. The DOE indicated that the current revision of the precipitates/salts report does not contain additional technical bases. The NRC questioned whether the current results were bounding, considering that experiments with introduced materials had not yet been completed. The DOE responded that the chemical divide effect is the biggest influence in determining final

compositions. The DOE noted plans to make comparisons to results of kinetic models. The NRC noted that mineral precipitates observed in evaporation tests were few compared to modeled precipitates. The DOE responded that precipitates may not be detectable and that solution composition variations may reveal precipitation. However, the DOE noted that some predicted precipitates should have been detectable. The NRC questioned the validity of equilibrium modeling for silica and the DOE acknowledged that silica is a difficult species to model at equilibrium. Mr. Don Shettel (Nye County) asked if thermal gradient tests were being conducted to test for coupled nonequilibrium phenomena. The DOE responded that thermal gradient tests were being examined for model validation purposes.

Subissue 2: Range of Water Chemistry and Trace Elements in the Waste Package Chemical Environment

The fourth DOE presentation (see "Subissue 2: Range of Water Chemistry and Trace Elements in the Waste Package Chemical Environment" presentation given by Gregory Gdowski) addressed two NRC concerns. The first NRC concern is that the DOE should provide information on the full water chemistry, including trace metals important to drip shield and waste package performance. The second NRC concern is that the DOE should provide additional laboratory and field data on the performance of the drip shield, especially in the presence of fluoride. The DOE identified the processes, in existing models, that control the chemistry of water contacting the waste packages. The type of brine characterization studies that the DOE has conducted and has planned to conduct was then described. The DOE presented information on the various sources for the water chemistry information, including thermal tests and laboratory aqueous solutions. The NRC asked whether the DOE had any plans to characterize dust that might settle on engineered materials. The DOE described that both air sampling and wipe tests would be conducted. Mr. Carl DiBella (NWTRB staff) asked whether the dust would be evaluated for organic components (e.g., pollen, spores) and the DOE stated that the sampled dust would be characterized by scanning electron microscopy. Plans to analyze laboratory solutions that have interacted with introduced materials were presented by the DOE. The types of information collected from the various field and laboratory experiments were identified. The NRC noted that it needs documentation of the rationale that the DOE used to select only a limited subset of water sample analyses in the Drift Scale Heater Test to calibrate or validate its model of coupled THC processes. The NRC asked whether and where the results from the Atlas facility crushed tuff experiments were documented. The DOE indicated that results were not yet documented.

Results from evaporative concentration tests that used a bicarbonate-type water and chloride-sulfate-type water were presented. The NRC staff questioned whether these results supported the assumption of chemical equilibrium. The relationship of the time scale of the experiments to the time steps used in performance assessment calculations was also questioned by the NRC. The NRC staff questioned whether the DOE understands the water chemistry at the time of initial re-wetting of the completely dry precipitates. The NRC also noted that two types of water tested could adversely impact different barriers and asked how the DOE would choose which type of water chemistry to use in performance assessment calculations. Finally, the NRC questioned whether the DOE will complete evaporative concentration experiments with solutions that had initially reacted with engineered materials. The DOE indicated that these tests are being considered.

Trace element concentrations were provided for J-13 and EJ-13 water samples. Mr. Don Shettle (Nye County) asked whether trace elements in the corrosion tests would be measured. Information on plans to characterize the trace element content of solutions used in the long-term corrosion testing program was provided by DOE. The NRC asked whether speciation of trace elements like lead was going to be measured in the trace element tests. The DOE replied that it was not currently in the scope of the planned work. Finally, the DOE described the type of testing being conducted for the Ti Grade 7 drip shield, including testing that will incorporate elevated levels of fluoride in dilute waters. The NRC questioned whether waters would have around 1000 ppm of fluoride and whether the DOE knows what the consequences would be for drip shield performance. The DOE indicated that the elevated range of fluoride would encompass 1000 ppm and that the consequences to drip shield performance have not yet been quantified.

Subissue 2: NRC Comments on Data Uncertainties and Sensitivity Studies

The fifth DOE presentation (see "Subissue 2: NRC Comments on Data Uncertainties and Sensitivity Studies" presentation given by Ernest Hardin) addressed three NRC concerns. The first NRC concern is that data uncertainties should be evaluated more rigorously in the DOE Physical and Chemical Environment model analysis/model reports. The DOE summarized the technical basis for resolution, described the technical basis for their current approach, and described planned actions to further support existing models. The DOE is relying on model improvements, more extensive use of natural and man-made analogs, and the corrosion testing process to address limitations associated with validating EBS models of the physical and chemical environment. The DOE is addressing data uncertainties by comparing predicted equilibrium conditions to test data in experiments that may not produce equilibrium conditions. The DOE asserted that data uncertainties are addressed by using a plausible boundary condition, however they also indicated ongoing work will evaluate alternatives. The NRC indicated that the compositions used may not be bounding.

The second NRC concern is that additional sensitivity studies should be performed by the DOE to identify the limitations of models used to predict coupled THC processes, and the evolution of water and gas compositions with time. The DOE presented four lines of evidence to support resolution of the sensitivity study concern. First, the DOE is comparing results obtained with the abstracted THC model to the J-13 and matrix pore water compositions that are also used for influent water. The NRC expressed a concern that unless the conditions under which the data have been collected are sufficiently described, it is unlikely that the range of uncertainty can be adequately assessed. In addition, the NRC indicated that the data that are currently being used for model calibration or model support have not been rigorously addressed in terms of its uncertainty (e.g., analytical, sampling). Second, steel corrosion rates are evaluated with different water compositions to estimate the possible range of corrosion rates. Third, the DOE asserted that effects of drift seepage on the in-drift thermodynamic environment (relative humidities and temperatures) are minor. Finally, mixing and disperison of gas-phase constituents produced and consumed in the drifts, associated with thermal-hydrologic circulation in the host rock are being evaluated.

The final concern addressed (also see "Addendum to Data Uncertainties and Sensitivity Studies Presentation for Subissue 2: Validation Approach for the Precipitates/Salts Model" presented by Ernest Hardin) was that the DOE has insufficiently validated the Physical and Chemical Environment models, including the critical evaluation of data used in model validation. The

DOE indicated that they are focusing on data and model issues with the greatest potential to affect repository performance. For instance, the DOE is considering developing additional laboratory test data to constrain the interpolative Low Relative Humidity Salts Model. The NRC stated that this model has not been adequately validated. The DOE also indicated additional sensitivity testing will be performed for planned report revisions. Comparison of the Precipitates/salts Model results using the PT4 database to calculations from the Harvie, Moeller, Weare database for a Canadian Shield Brine and a Dead Sea Brine at ambient temperatures were presented. The DOE presented a comparison of lab test data from the evaporative concentration experiments at elevated temperatures to the PT4 predictions. The NRC indicated that those tests had mass balance problems which calls into question the usefulness of the comparison. The DOE indicated that they planned to repeat the tests. Agreement between the models was good, except for nitrate salts. In addition the PT4 results were compared to handbook aqueous solubilities for sodium and potassium salts at 100°C. The DOE described the uncertainties of the elevated temperature data used in the comparisons. The NRC indicated that the DOE only needed to validate those activities that were used to address corrosion in the performance assessment calculations. However, the information that compared predicted solid phases to the observed solid phases suggests that the predictions are inaccurate. The DOE described the physical characterization, by use of X-ray diffraction techniques, of the evaporated salts. The DOE agreed with the NRC observation that solid phases that were not subject to dissolution from changes of relative humidity were not observed in the sample, even though detection limits should have allowed their observation. The DOE suggested that this type of question is being evaluated in ongoing and planned activities. The NRC asked whether both the reduced and extended mineral models used in the Drift-Scale THC model were going to be validated. The DOE indicated that efforts to validate both models would be documented in a revised report.

ENFE Subissue 2 Overall Status

As a result of additional discussions, the NRC and DOE reached 18 agreements for Subissue #2 (see Attachment 1). With these 18 agreements, the NRC stated that Subissue #2 could be listed as "closed-pending."

6) Technical Discussion - Subissue #3, Effects of Coupled Thermal-Hydrologic-Chemical Processes on the Chemical Environment for Radionuclide Release

Subissue 3: NRC Comments on Thermal-Hydrological-Chemical Effects on Radionuclide Release

A summary of the current status of resolution was presented (see "Subissue 3: NRC Comments on Thermal-Hydrological-Chemical Effects on Radionuclide Release" presentation given by Christine Stockman). This presentation addressed 14 NRC comments (comments regarding colloids were addressed earlier in the meeting in the presentation titled "Subissue 3: NRC Comments Related to Total System Performance Assessment for the Site Recommendation Results Related Waste Form Degradation.") The DOE answered the comments with references to analyses documented in a number of DOE reports and to planned activities. Comments concerning the DOE neglect of high-temperature effects such as evaporative concentration of chloride and fluoride were answered with the assertion that no seepage would enter the waste package during the thermal period. The DOE's analyses does not currently predict failures of the waste package within the 10,000 year regulatory time period. The NRC

believes the release models applicable for early waste package failure when chemical conditions may be perturbed may need to be considered in multiple barrier analyses; this topic is expected to be addressed in the TSPAI technical exchange. Also, the DOE argued that evaporative concentration of fluoride is unimportant because they assume that all fluoride entering the waste package is utilized in cladding corrosion. The NRC pointed out that this is not necessarily conservative with respect to peak mean dose. The NRC commented that not all DOE arguments concerning degradation rates for spent nuclear fuel were strong, but that the modeled rates were nonetheless sufficiently conservative. The NRC asked how uncertainties arising from temperature dependence of thermodynamic parameters were handled. The DOE responded that new sensitivity studies are under consideration. NRC concerns regarding the neglect of local chemical environments were raised. The NRC returned to comments on colloid release modeling first discussed in the presentation titled "Subissue 3: NRC Comments Related to Total System Performance Assessment for the Site Recommendation Results Related Waste Form Degradation." The DOE pointed to a report on radionuclide selection that contained information on those radionuclides for which colloidal release was modeled. Regarding the NRC question on the DOE neglect of commercial spent nuclear fuel (CSNF) colloid production, the DOE described how CSNF corrosion tests are being altered to promote the detection of any colloids. On the use of the lab corrosion test results in the colloidal release abstraction, the DOE indicated that additional discussion of some of the uncertainties, assumptions, and alternative models would be included in a future revision of the AMR titled "Waste Form Colloid-Associated Concentration Limits: Abstraction and Summary."

As a result of additional discussions, the NRC and DOE reached 5 agreements for Subissue #3 (see Attachment 1). With these 5 agreements, the NRC stated that Subissue #3 could be listed as "closed-pending."

7) Features, Events, and Processes

The DOE presented information on FEPs during the Thermal Effects on Flow KTI meeting held on January 8-9, 2001 (see "Features, Events, and Processes for Thermal Effects on Flow and Evolution of the Near Field Environment" presentation given by Nicholas Francis). The NRC questioned whether the FEPs AMR updates would address all the NRC comments in Revision 3 of the IRSRs, including whether traceable references for the documentation of low consequence calculations will be provided. The DOE stated that it believed many of the NRC comments were addressed and requested that the NRC review the updates and provide the DOE with any additional comments. The DOE also provided a summary of the TEF and ENFE FEPs.

8) Public Comments

In addition to the public questions and comments mentioned above, Ms. Judy Treichel (Nevada Nuclear Waste Task Force) addressed the uncertainties apparent from the discussions at the meeting concerning the interpretation of the results from the drift-scale heater test. She noted that visitors to the test facility are left with the impression that the test is a better simulation of the repository than it actually is. Declaring related subissues as "closed-pending" implies a level of comfort in interpreting drift-scale heater test results that is higher than is apparent from this meeting. Ms. Treichel also commented (1) that she was uncomfortable with the DOE reliance on a 10,000-year container lifetime for its safety case, and did not think members of the public would be convinced of its validity, and (2) that she disapproved of the use of the

"closed-pending" issue label. She feels that the label is artificial and has the psychological effect of suggesting that the DOE has proven its case, despite the fact that years of studies are yet to be conducted.

Mr. Don Shettel (Nye County) questioned the DOE's model results showing only minor mineral precipitation in host rocks during the thermal period, with resulting minor predicted changes in porosity and permeability. He pointed out that in natural refluxing zones, mineral precipitation in boiling zones and dissolution in condensate zones is common. The DOE responded that the experiments that show large effects are designed favorably for precipitation and so may not be applicable. Mr. Shettel responded that perhaps the drift-scale test design is not favorable for promoting precipitation. Mr. Shettel also stated that as a consultant to Nye County, his primary objective is protecting the health and safety of Nye County residents. He feels that only the best science should be applied in meeting that goal. He asked attendees to consider his earlier questions in that light.

1/12/01

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HLW Branch Chief
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1/12/2001

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Summary of the Resolution of the Key Technical Issue on Evolution of the Near-Field Environment

Subissue #	Subissue Title	Status	NRC/DOE Agreements
1	Effects of coupled thermal-hydrologic-chemical processes on seepage and flow	Closed-Pending	1) Provide updated FEPs AMRs with additional technical bases for those FEPs previously identified by the NRC in Rev. 03 of the ENFE IRSR as inadequately screened. In Rev 03 of the ENFE IRSR, the NRC identified 17 FEPs associated with Subissue 1 for which no screening arguments were identified in the FEPs data base, screening arguments were inconsistent with other project documents, or inadequate exclusion arguments were provided. The lack of screening arguments has been addressed in Rev 00 of the FEPs data base and Rev 00 of the supporting AMRs. Current revisions (or ICNs) of the FEPs AMRs, scheduled for completion in January 2001, will partially address the remaining NRC comments. Consideration of the remaining NRC comments will be provided in subsequent FEPs AMR revisions, expected to be available as periodic revisions, the entirety of which will be available prior to license application. 2) Provide the FEPs database. The DOE will provide the FEPs data base to the NRC during March 2001.

1	Effects of coupled thermal-hydrologic-chemical processes on seepage and flow - cont.		3) Provide the Drift-Scale Coupled Processes (DST and THC Seepage) Models AMR, Rev. 01 and 02, including (1) information on the quantity of unreacted solute mass that is trapped in dry-out zone in TOUGHREACT simulations, as well as how this would affect precipitation and the resulting change in hydrologic properties and (2) documentation of model validation consistent with the DOE QA requirements. The DOE will provide documentation of model validation, consistent with the DOE QA requirements, in the *Drift-Scale Coupled Processes (DST and THC Seepage) Models* AMR (MDL-NBS-HS-000001) Rev 01, expected to be available to the NRC in March 2001. The DOE will provide information on the quantity of unreacted solute mass that is trapped in the dryout zone in TOUGHREACT simulations in the *Drift-Scale Coupled Processes (DST and THC Seepage) Models* AMR Rev 02, expected to be available to the NRC in FY 02. 4) Provide additional technical bases for the DOE's treatment of the effects of cementitious materials on hydrologic properties. The DOE will provide additional information on the effects of cementitious materials in an update to the *Unsaturated Zone Flow and Transport* PMR (TDR-NBS-HS-000002), available in FY 02. Information provided will include results of evaluation of the magnitude of potential effects on hydrologic properties and radionuclide transport characteristics of the unsaturated zone. 5) Address the various sources of uncertainty (e.g., model implementation, conceptual model, and data uncertainty (hydrologic, thermal, and geochemical)) in the THC model. The DOE will evaluate the various sources of uncertainty in the THC process model, including details as to how the propagation of various sources of uncertainty are calculated in a systematic uncertainty analysis. The DOE will document that uncertainty evaluation in the *Drift-Scale Coupled Processes (DST and THC Seepage) Models* AMR (MDL-NBS-HS-000001) Rev 02 (or in another future document), expected to be available in FY 02.

1	Effects of coupled thermal-hydrologic-chemical processes on seepage and flow - cont.		6) Provide the technical basis for excluding entrained colloids in the analysis of FEP 2.2.10.06.00 (Thermo-Chemical Alteration) or an alternative FEP. The DOE will provide the technical basis for screening entrained colloids in the analysis of FEP 2.2.10.06.00 in a future revision of the *Features, Events, and Processes in UZ Flow and Transport* AMR (ANL-NBS-MD-000001), expected to be available in FY 02. 7) Provide physical evidence that supports the model of matrix fracture interaction precipitation effects (e.g., coring). The DOE will provide the following evidence that supports the model of matrix/fracture interaction precipitation effects: (1) Existing data from the Single Heater Test (SHT) of post-test overcoring Mineralogy-Petrology (Min-Pet) analysis (SHT final report [MOL.20000103.0634] and DTN LASL831151.AQ98.001) is expected to be provided to the NRC in March 2001. (2) Results of ongoing side-wall sampling Min-Pet analyses of DST samples are expected to be provided to the NRC in FY 02. (3) The DOE expects to provide the *Drift-Scale Coupled Processes (DST and THC Seepage) Models* AMR (MDL-NBS-HS-000001) Rev 01 to the NRC as evidence of matrix-fracture interaction in March 2001.
2	Effects of coupled thermal-hydrologic-chemical processes on waste package chemical environment	Closed-Pending	1) Provide updated FEPs AMRs with additional technical bases for those FEPs previously identified by the NRC in Rev. 03 of the ENFE IRSR as inadequately screened. In Rev 03 of the ENFE IRSR, the NRC identified 24 FEPs associated with Subissue 2 for which no screening arguments were identified in the FEPs data base, screening arguments were inconsistent with other project documents, or inadequate exclusion arguments were provided. The lack of screening arguments has been addressed in Rev 00 of the FEPs data base and Rev 00 of the supporting AMRs. Current revisions (or ICNs) of the FEPs AMRs, scheduled for completion in January 2001, will partially address the remaining NRC comments. Consideration of the remaining NRC comments will be provided in subsequent FEPs AMR revisions, expected to be available as periodic revisions, the entirety of which will be available prior to license application. 2) Provide the FEPs database. The DOE will provide the FEPs data base to the NRC during March 2001.

2	Effects of coupled thermal-hydrologic-chemical processes on waste package chemical environment - cont.		3) Provide the technical basis for FEP 1.2.06.00 (Hydrothermal Activity), addressing points (a) through (e) of NRC Subissue 2 slide handed out at the January 2001 ENFE technical exchange. The DOE will provide additional technical bases for the screening of FEP 1.2.06.00 (Hydrothermal Activity), in a future revision of the *Features, Events, and Processes in UZ Flow and Transport* AMR (ANL-NBS-MD-000001), expected to be available in FY 02. Within these technical bases, the DOE will address NRC comments [points (a) through (e)] presented on the NRC Subissue 2 slide handed out at the January 2001 ENFE technical exchange or provide justification that it is not needed. 4) Provide the technical basis for bounding the trace elements and fluoride for the geochemical environment affecting the drip shield and waste package, including the impact of engineered materials. The DOE will document the concentrations of trace elements and fluoride in waters that could contact the drip shield and waste package in a revision to the *Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier* AMR (ANL-EBS-MD-000001), which will be available in FY02. In addition, trace elements and fluoride concentrations in introduced materials in the EBS (including cement grout, structural steels, and other materials as appropriate) will be addressed in a revision to the *Engineered Barrier System: Physical and Chemical Environment Model AMR* (ANL-EBS-MD-000033), expected to be available in FY 02. 5) Evaluate data and model uncertainties for specific in-drift geochemical environment submodels used in TSPA calculations and propagate those uncertainties following the approach described in Agreement #5, Subissue 1. The DOE will evaluate data and model uncertainties for specific in-drift geochemical environment submodels used in TSPA calculations and propagate those uncertainties following the approach described in Subissue 1, Agreement #5. The DOE will document the evaluation in an update to the *Engineered Barrier System: Physical and Chemical Environment Model* AMR (ANL-EBS-MD-000033) (or in another future document), expected to be available in FY 02.

2	Effects of coupled thermal-hydrologic-chemical processes on waste package chemical environment - cont.		6) Evaluate the impact of the range of local chemistry (e.g., dripping of equilibrated evaporated cement leachate and corrosion products) conditions at the drip shield and waste package considering the chemical divide phenomena that may propagate small uncertainties into large effects. The DOE will evaluate the range of local chemical conditions at the drip shield and waste package (e.g. local variations in water composition associated with cement leaching or the presence of corrosion products), considering potential evaporative concentration and the chemical divide effect whereby small differences in initial composition could cause large differences in brine characteristics. This evaluation will be documented in a revision to the *Engineered Barrier System: Physical and Chemical Environment Model* AMR (ANL-EBS-MD-000033), expected to be available in FY 02. 7) Identify specific coupling relationships that are included and excluded from TSPA, including Onsager couples, and give technical bases for their inclusion or exclusion. The DOE will identify specific coupling relationships that are included and excluded from TSPA, including Onsager couples, and give the technical basis for inclusion and exclusion. This information will be documented in a revision to the *Engineered Barrier System Degradation, Flow, and Transport* PMR (TDR-EBS-MD-000006), expected to be available by September 2001. 8) Provide stronger technical basis for the suppression of individual minerals predicted by equilibrium models. The DOE will provide additional technical basis for suppression of individual minerals predicted by equilibrium models, in a revision to the *Engineered Barrier System: Physical and Chemical Environment Model* AMR (ANL-EBS-MD-000033), expected to be available in FY02.

2	Effects of coupled thermal-hydrologic-chemical processes on waste package chemical environment - cont.		9) Provide the In-Drift Precipitates/Salts Analysis AMR, Rev. 00, ICN 02, including (1) the major anionic (e.g., fluoride or chloride) and cationic species, and (2) additional technical basis for the low relative humidity model. The DOE will provide the *In-Drift Precipitates/Salts Analysis* AMR (ANL-EBS-MD-000045), Rev. 00, ICN 02, including the major anionic (e.g., fluoride or chloride) and cationic species, in January 2001. The DOE will provide to the NRC an update to the *In-Drift Precipitates/Salts Analysis* AMR (ANL-EBS-MD-000045) that will provide additional technical bases for the low relative humidity model, expected to be available in FY 02. 10) Provide additional information about the range of composition of waters that could contact the drip shield or waste package, including whether such waters are of the bicarbonate or chloride-sulfate type. The DOE will describe the range of bulk composition for waters that could affect corrosion of the drip shield or waste package outer barrier, in a revision to the *Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier* AMR (ANL-EBS-MD-000001), expected to be available in FY02. 11) Provide the technical basis for the current treatment of the kinetics of chemical processes in the in-drift geochemical models. This basis should address data in the figure on page 16 of the G.Gdowski Subissue 2 presentation with appropriate treatment of time as related to abstractions used in TSPA. The DOE will provide additional technical basis for the treatment of precipitation-dissolution kinetics by the in-drift geochemical models, in a revision to the *Engineered Barrier System: Physical and Chemical Environment Model* AMR (ANL-EBS-MD-000033), expected to be available in FY02. The technical basis will include reaction progress simulation for laboratory evaporative concentration tests, and will include appropriate treatment of time as related to the residence times associated with the abstractions used to represent in-drift processes in TSPA.

2	Effects of coupled thermal-hydrologic-chemical processes on waste package chemical environment - cont.		12) Provide the documentation and analysis of the column crush tuff experiments. The DOE will provide documentation of the results obtained from the crushed tuff hydrothermal column experiment, and of post-test analysis, in new reports specific to the column test, expected to be available by September 2001. 13) Provide documentation regarding the deposition of dust and its impact on the salt analysis. The DOE will provide documentation of dust sampling in the Exploratory Studies Facility, and analysis of the dust and evaluation of its impact on the chemical environment on the surface of the drip shield and waste package, in a revision to the *Engineered Barrier System: Physical and Chemical Environment Model* AMR (ANL-EBS-MD-000033), expected to be available in FY02. 14) Provide the analysis of laboratory solutions that have interacted with introduced materials. The DOE will provide additional information about laboratory solutions that have interacted with introduced materials, in a revision to the *Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier* AMR (ANL-EBS-MD-000001), expected to be available in FY02. 15) Provide the additional data to constrain the interpolative low relative humidity salts model. The data should provide the technical basis as to why the assumption of the presence of sodium nitrate is conservative, when modeling and experimental results indicate the presence of other mineral phases for which the deliquesence point is unknown. The DOE will provide additional information to constrain the low-relative humidity salts model. The information will include the deliquescence behavior of mineral assemblages derived from alternative starting water compositions (including bulk water compositions, and local variations associated with cement leaching or the presence of corrosion products) representing the range of potential water compositions in the emplacement drifts. This information will be documented in a revision to the *In-Drift Precipitates/Salts Analysis* AMR (ANL-EBS-MD-000045), expected to be available in FY02.
2	Effects of coupled		16) Provide the Drift-Scale Coupled Processes (DST and THC Seepage)

	thermal-hydrologic-chemical processes on waste package chemical environment - cont.		Models, Rev. 01, including information supporting both the limited suite mineral model and the more complete extended model. The DOE will provide the *Drift-Scale Coupled Processes (DST and THC Seepage) Models* AMR (MDL-NBS-HS-000001) Rev 01, including information supporting both the limited suite mineral model and the more complete extended model, in March 2001. 17) Provide documentation of data used to calibrate models and data to support model predictions, and an assessment of data uncertainty (e.g., sampling and analytical), that includes critical analyses of variables that affect the data measurements and their interpretations (e.g., drift-scale thermal test and evaporation tests). The DOE will provide documentation of data used to calibrate models and data to support model predictions, and an assessment of data uncertainty (e.g., sampling and analytical) in the area of water and gas chemistry from the drift-scale thermal tests and evaporation tests. This documentation will be provided in revisions to the following AMRs: *Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier* (ANL-EBS-MD-000001), *Engineered Barrier System: Physical and Chemical Environment Model* (ANL-EBS-MD-000033), and *Drift-Scale Coupled Processes (DST and THC Seepage) Models* (MDL-NBS-HS-000001), or other documents as appropriate. All documents or revisions are expected to be available in FY 02. 18) Provide the following documents: EBS: Physical and Chemical Environment Model, Rev. 01; Multiscale Thermohydrologic Model, Rev. 00, ICN 01; Abstraction of Drift-Scale Coupled Processes, Rev 01; Environments on the Surfaces of the Drip Shield and the Waste Package Outer Barrier, Rev. 00, ICN 01; Waste Package Degradation PMR, Rev. 00, ICN 01; EBS Degradation, Flow, and Transport PMR, Rev. 01; Near Field Environment PMR, Rev. 00, ICN 02 and Rev. 01; Hydrogen Induced Cracking of Drip Shield, Rev. 00, ICN 01; Drift Degradation Analysis, Rev. 01; Design Analysis for the Ex-Container Components, Rev. 00; Longevity of Emplacement Drift Ground Support Materials, Rev. 01; Stress Corrosion Cracking AMR, Rev. 00, ICN 01; In-Drift Microbial Communities, Rev. 00, ICN 01; Physical and Chemical Environment Abstraction Model, Rev. 00, ICN 01; UZ Flow and Transport Model PMR, Rev. 01; General Corrosion and Localized Corrosion

			of the Drip Shield, Rev. 00; Water Distribution and Removal Model, Rev. 01. The DOE will provide the documents requested by the dates indicated: *Engineered Barrier System: Physical and Chemical Environment Model* (ANL-EBS-MD-000033) Rev. 01: FY 02; *Multiscale Thermohydrologic Model* (ANL-EBS-MD-000049) Rev. 00, ICN 01: January 2001; *Abstraction of Drift-Scale Coupled Processes* (ANL-NBS-HS-000029) Rev 01: September 2001; *Environment on the Surfaces of the Drip Shield and the Waste Package Outer Barrier* (ANL-EBS-MD-000001) Rev. 00, ICN 01: January 2001; *Waste Package Degradation* PMR (TDR-WIS-MD-000002) Rev. 00, ICN 01: January 2001; *Engineered Barrier System Degradation, Flow, and Transport* PMR (TDR-EBS-MD-000006) Rev. 01: September 2001; *Near Field Environment* PMR (TDR-NBS-MD-000001) Rev. 00, ICN 02: January 2001 and Rev. 01: September 2001; *Hydrogen Induced Cracking of Drip Shield* (ANL-EBS-MD-000006) Rev. 00, ICN 01: January 2001; *Drift Degradation Analysis* (ANL-EBS-MD-000027) Rev. 01: January 2001; *Design Analysis for the Ex-Container Components*, ANL-XCS-ME-000001 Rev. 00: January 2001; *Longevity of Emplacement Drift Ground Support Materials* (ANL-EBS-GE-000003) Rev. 01: January 2001; *Stress Corrosion Cracking* of the Drip Shield, the Waste Package Outer Barrier, and the Stainless Steel Structural Material AMR (ANL-EBS-MD-000005) Rev. 00, ICN 01: January 2001; *In-Drift Microbial Communities* (ANL-EBS-MD-000038) Rev. 00, ICN 01: January 2001; *Physical and Chemical Environmental Abstraction Model* (ANL-EBS-MD-000046) Rev. 00, ICN 01: January 2001; *Unsaturated Zone Flow and Transport Model* PMR (TDR-NBS-HS-000002) Rev. 01: September 2001; *General Corrosion and Localized Corrosion of the Drip Shield* (ANL-EBS-MD-000004) Rev. 00: January 2001; *Water Distribution and Removal Model* (ANL-EBS-MD-000032) Rev. 01: January 2001.

3	Effects of coupled thermal-hydrologic-chemical processes on chemical environment for radionuclide release	Closed-Pending	1) Provide the following documents: WAPDEG Analysis of Waste Package and Drip Shield Degradation AMR, Rev. 00, ICN 01; Near-Field Environment PMR, Rev. 00, ICN 03; In-Package Chemistry AMR, Rev. 01; CAL-EBS-PA-000002, Rev. 01; ANL-EBS-PA-000005, Rev. 00; In-Package Chemistry Abstraction AMR, Rev. 01; TSPA-SR, Rev. 00; Waste Form Colloid-Associated Concentration Limits: Abstraction and Summary AMR. The DOE will provide the following documents to the NRC by February 2001: *WAPDEG Analysis of Waste Package and Drip Shield Degradation* AMR (ANL-EBS-PA-000001) Rev 00 ICN 01; *Near Field Environment* PMR (TDR-NBS-MD-000001) Rev 00 ICN 03; *Summary of In-Package Chemistry for Waste Forms* AMR (ANL-EBS-MD-000050) Rev 01; *Calculation of General Corrosion Rate of Drip Shield and Waste Package Outer Barrier to Support WAPDEG Analysis* (CAL-EBS-PA-000002) Rev 01; *Abstraction of Models for Stainless Steel Structural Material Degradation* (ANL-EBS-PA-000005) Rev 00; *In-Package Chemistry Abstraction* AMR (ANL-EBS-MD-000037) Rev 01; *Total System Performance Assessment for the Site Recommendation* (TDR-WIS-PA-000001) Rev 00; *Waste Form Colloid-Associated Concentrations Limits: Abstraction and Summary* AMR (ANL-WIS-MD-000012) Rev 00 ICN 01 2) Provide the thermodynamic database and the report associated with the database. The DOE will provide the thermodynamic data base [Input Transmittal for Thermodynamic Data Input Files for Geochemical Calculations (MO0009THRMODYN.001)] and *Data Qualification Report for the Thermodynamic Data File, DATA0.ympR0 for Geochemical Code EQ 3/6* (TDR-EBS-MD-000012) to the NRC in February 2001. 3) Provide analyses to verify that bulk-scale chemical processes dominate the in-package chemical environment. The DOE will provide analyses justifying the use of bulk chemistry as opposed to local chemistry for solubility and waste form degradation models. These analyses will be documented in an update to the *Miscellaneous Waste-Form FEPs* AMR (ANL-WIS-MD-000009) or in an update to the *Summary of In-Package Chemistry for Waste Forms* AMR (ANL-EBS-MD-000050), expected to be available in FY 02.

3	Effects of coupled thermal-hydrologic-chemical processes on chemical environment for radionuclide release - cont.		4) Complete validation of in-package chemistry models. Agreement #5 for CLST subissue 3 addresses testing plans. Model validation based on this testing and further analysis will be documented in an update to the *Summary of In-Package Chemistry for Waste Forms* AMR (ANL-EBS-MD-000050), expected to be available in FY 02. 5) Provide the technical basis for selection of radionuclides that are released via reversible and irreversible attachment to colloids for different waste forms in the TSPA. The technical bases for the selection of radionuclides released via reversible and irreversible attachments to colloids for different waste forms is provided in section 3.5.6.1 of the *Total System Performance Assessment (TSPA) Model for Site Recommendation* (MDL-WIS-PA-000002) Rev 00. This document will be provided to the NRC in January 2001.
4	Effects of coupled thermal-hydrologic-chemical processes on radionuclide transport through engineered and natural barriers	Closed-Pending	1) Provide the executable version of the most recently qualified version of TOUGHREACT. The DOE will provide the executable TOUGHREACT Rev 2.2 to the NRC by February 2001, subject to the NRC obtaining any applicable agreement for usage of the software. 2) Provide the Drift-Scale Coupled Processes (DST and THC Seepage) Models AMR, Rev. 01 and 02. The DOE will provide the *Drift-Scale Coupled Processes (DST and THC Seepage) Models* AMR (MDL-NBS-HS-000001) Rev 01 to the NRC in March 2001. The DOE will provide the *Drift-Scale Coupled Processes (DST and THC Seepage) Models* AMR Rev 02 to the NRC in FY 02. 3) Provide the technical bases for screening out coupled THC effects on radionuclide transport properties and colloids. The DOE will provide the technical bases for screening out coupled THC effects on radionuclide transport properties and colloids in a new AMR or in a revision to an existing AMR, expected to be available in FY 02.

4	Effects of coupled thermal-hydrologic-chemical processes on radionuclide transport through engineered and natural barriers - cont		4) Provide the technical basis for excluding entrained colloids in the analysis of FEP 2.2.10.06.00 (Thermo-Chemical Alteration) or an alternative FEP. The DOE will provide the technical basis for screening entrained colloids in the analysis of FEP 2.2.10.06.00 in a future revision of the *Features, Events, and Processes in UZ Flow and Transport* AMR (ANL-NBS-MD-000001), expected to be available in FY 02. 5) Provide the screening criteria for the radionuclides selected for PA. Provide the technical basis for selection of radionuclides that are transported via colloids in the TSPA. The screening criteria for radionuclides selected for TSPA are contained in the AMR *Inventory Abstraction* (ANL-WIS-MD-000006) Rev 00, ICN 01. The DOE is documenting identification of radionuclides transported via colloids for TSPA in the AMR *Colloid-Associated Concentration Limits: Abstraction and Summary* (ANL-WIS-MD-000012) Rev 0, in the Total System Performance Assessment for the Site Recommendation (TDR-WIS-PA-000001) Rev 00 ICN 01, and in the *Total System Performance Assessment (TSPA) Model for Site Recommendation* (MDL-WIS-PA-000002) Rev 00. These documents will be available to the NRC in January 2001. 6) Provide documentation to demonstrate suitability of the bounding values used for colloid transport through the perturbed near-field environment. For example, consider sensitivity analyses to investigate the effects of varying colloid sorption parameters (K_c) on repository performance. The DOE will evaluate the suitability of the colloid transport model under perturbed conditions as discussed in agreement #3 for this subissue. As part of this work, the DOE will consider sensitivity analyses to investigate the effects of varying colloid sorption parameters (K_c) on repository performance. The DOE will also provide the TSPA-SR (TDR-WIS-PA-000001) Rev 00 ICN 01 in January 2001. The TSPA-SR includes sensitivity studies in the form of barrier degradation and parameter sensitivity analyses that investigate the effect of sorption and colloid parameters on repository performance.

4	Effects of coupled thermal-hydrologic-chemical processes on radionuclide transport through engineered and natural barriers - cont.		7) Provide updated FEPs AMRs with additional technical bases for those FEPs previously identified by the NRC in Rev. 03 of the ENFE IRSR as inadequately screened. In Rev 03 of the ENFE IRSR, the NRC identified 17 FEPs associated with Subissue 1 for which no screening arguments were identified in the FEPs data base, screening arguments were inconsistent with other project documents, or inadequate exclusion arguments were provided. The lack of screening arguments has been addressed in Rev 00 of the FEPs data base and Rev 00 of the supporting AMRs. Current revisions (or ICNs) of the FEPs AMRs, scheduled for completion in January 2001, will partially address the remaining NRC comments. Consideration of the remaining NRC comments will be provided in subsequent FEPs AMR revisions, expected to be available as periodic revisions, the entirety of which will be available prior to license application. 8) Provide the FEPs database. The DOE will provide the FEPs data base to the NRC during March 2001.

DOE-NRC TECHNICAL EXCHANGE AGENDA THERMAL EFFECTS ON FLOW AND EVOLUTION OF THE NEAR-FIELD ENVIRONMENT KEY TECHNICAL ISSUES **January 8-12, 2001** **Pleasanton, California**			
Monday, January 8, 2001			
Schedule	TEF Presentation	Time (Minutes)	
		Duration	Discussion
8:00 – 8:20 AM	Introduction/Objectives (DOE-NRC)	20	
8:20 – 8:40 AM	TEF Summary (Barr)	10	10
8:40 – 9:10 AM	Uncertainties (Coppersmith)	20	10
9:10 – 9:45 AM	TSPA for TEF (Francis)	20	15
9:45 – 10:00 AM	BREAK	15	
10:00 – 10:30 AM	TEF and ENFE FEPs (Francis)	15	15
10:30 – 11:15 AM	Caucus Subissue 1		45
11:15 – 11:45 AM	DOE-NRC Discussion of Resolution Status		30
11:45 AM – 12:45 PM	LUNCH	60	
12:45 – 4:15 PM with 15-minute break	Subissue 2 Open Item Presentations		
	Open Item 1: Repository Design (Hardin)	15	10
	Open Item 2: Cold Traps (Hardin)	15	10
	Open Item 6: Ventilation Model (Hardin)	15	10
	Open Item 5: Cross Drift Thermal Testing (Peters)	20	10
	Open Item 7: Data Uncertainty (Bodvarsson)	30	15
	Open Item 8: Model Uncertainty (Bodvarsson)	30	15
4:15 – 5:15 PM	Caucus Subissue 2	60	
5:15 – 5:45 PM	DOE-NRC Discussion of Resolution Status		30
5:45 – 6:00 PM	Closing Remarks	15	
6:00 PM	Adjourn Day 1		

DOE-NRC TECHNICAL EXCHANGE AGENDA
THERMAL EFFECTS ON FLOW AND EVOLUTION OF THE NEAR-FIELD ENVIRONMENT KEY TECHNICAL ISSUES
January 8-12, 2001
Pleasanton, California

Tuesday, January 9, 2001			
Schedule	TEF Presentation	Time (Minutes)	
		Duration	Discussion
8:00 – 9:00 AM	Final TEF Caucus		60
9:00 – 9:15 AM	Closing Remarks	15	
9:15 AM	Adjourn TEF Technical Exchange		
9:15 – 11:30 AM	Develop TEF Meeting Minutes and Agreement Letter	135	
11:30 – 11:45 AM	BREAK	15	

ENFE Technical Exchange			
Schedule	ENFE Presentation	Time (Minutes)	
		Duration	Discussion
11:45 AM – 12:05 PM	Introduction/Objectives (DOE-NRC)	20	
12:05 – 12:30 PM	ENFE KTI Summary (Barr)	15	10
12:30 – 1:30 PM	LUNCH	60	
1:30 – 4:10 PM (15-minute break)	ENFE TSPA Treatments and Impacts		
	EBS Chemical Environments (Nowak)	25	20
	TSPA-SR Results Related to Waste Form Degradation (Rechard)	25	25
	Effects of Coupled THC Processes on Radionuclide Transport (Gross)	25	20
4:10 – 4:50 PM	Subissue 1 Seepage and Flow: Coupled THC Processes Affecting CHn (Sonnenthal)	25	15
4:50 – 5:05 PM	Closing Remarks	15	
5:05 PM	Adjourn Day 2		

DOE-NRC TECHNICAL EXCHANGE AGENDA THERMAL EFFECTS ON FLOW AND EVOLUTION OF THE NEAR-FIELD ENVIRONMENT KEY TECHNICAL ISSUES **January 8-12, 2001** **Pleasanton, California**			
Wednesday, January 10, 2001			
Schedule	ENFE Presentation	Time (Minutes)	
		Duration	Discussion
8:00 – 10:30 AM (15-minute break)	Subissue 1: Seepage and Flow (Continued)		
	Thermal Alteration of PTn (Spycher)	25	15
	Effects of Cementitious Materials (Hardin)	25	15
	Mineral Precipitation in Fractures or at Fracture-Matrix Interface (Sonnenthal)	25	20
10:30 AM – Noon	Caucus on Subissue 1	90	
Noon – 1:00 PM	LUNCH	60	
1:00 – 1:30 PM	DOE-NRC Discussion of Resolution Status of Subissue 1		30
1:30 – 2:15 PM	Subissue 4 Item: Colloidal Transport in the UZ (Houseworth)	25	20
2:15 – 3:15 PM	Caucus on Subissue 4	60	
3:15 – 3:30 PM	BREAK	15	
3:30 – 4:00 PM	DOE-NRC Discussion of Resolution Status of Subissue 4		30
4:00 – 4:55 PM	Subissue 2 THC Effects on Waste Package Environment: In-Drift Geochemical Environment (Hardin)	30	25
4:55 – 5:10 PM	Closing Remarks	10	
5:10 PM	Adjourn Day 3		

DOE-NRC TECHNICAL EXCHANGE AGENDA
THERMAL EFFECTS ON FLOW AND EVOLUTION OF THE NEAR-FIELD ENVIRONMENT KEY TECHNICAL ISSUES
January 8-12, 2001
Pleasanton, California

Thursday, January 11, 2001			
Schedule	ENFE Presentation	Time (Minutes)	
		Duration	Discussion
8:00 – 11:15 AM (15-minute break)	Subissue 2 THC Effects on Waste Package Environment (Continued)		
	Treatment of Coupled Processes and Model Integration (Hardin)	30	15
	Assumption of Chemical Equilibrium (Hardin)	30	15
	Range of Water Chemistry and Trace Elements in the WP Chemical Environment (Gdowski)	30	15
	Data and Model Uncertainties and Sensitivity Studies (Hardin)	30	15
11:15 AM – 12:30 PM	Caucus on Subissue 2	75	
12:30 – 1:30 PM	LUNCH	60	
1:30 – 2:00 PM	DOE-NRC Discussion of Resolution Status of Subissue 2		30
2:00 – 3:20 PM	Subissue 3 THC Effects on Radionuclide Release (Stockman)	45	35
3:20 – 3:35 PM	BREAK	15	
3:35 – 4:35 PM	Caucus on Subissue 3	60	
4:35 – 5:05 PM	DOE-NRC Discussion of Resolution Status of Subissue 3		30
5:05 – 5:15 PM	Closing Remarks	15	
5:15 PM	Adjourn Day 4		

Friday, January 12, 2001			
8:00 AM – Noon	ENFE Meeting Minutes and Agreement Letter	240	

THERMAL EFFECTS ON FLOW AND EVOLUTION OF THE NEAR-FIELD ENVIRONMENT TECHNICAL EXCHANGE AND MANAGEMENT MEETINGS
JANUARY 8-11, 2001
PLEASANTON, CALIFORNIA

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ATTACHMENT 3

THERMAL EFFECTS ON FLOW AND EVOLUTION OF THE NEAR-FIELD ENVIRONMENT TECHNICAL EXCHANGE AND MANAGEMENT MEETINGS
JANUARY 8-11, 2001
PLEASANTON, CALIFORNIA

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THERMAL EFFECTS ON FLOW AND EVOLUTION OF THE NEAR-FIELD ENVIRONMENT TECHNICAL EXCHANGE AND MANAGEMENT MEETINGS
JANUARY 8-11, 2001
PLEASANTON, CALIFORNIA

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THERMAL EFFECTS ON FLOW AND
EVOLUTION OF THE NEAR-FIELD ENVIRONMENT
TECHNICAL EXCHANGE AND MANAGEMENT MEETINGS
JANUARY 8-11, 2001
PLEASANTON, CALIFORNIA

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ATTACHMENT 4

PRESENTER'S SLIDES

U.S. Nuclear Regulatory Commission: Evolution of Near Field Environment Key Technical Issue Subissue 2 Coupled Thermal-Hydrologic-Geochemical Effects on Waste Package Environment

NRC concern on the technical basis for treatment of FEP 1.2.06.00 (Hydrothermal activity).

NRC requires additional technical bases for its exclusion. If DOE chooses to exclude this FEP, DOE should:

A) Document the results (conductive cooling model of Timber Mountain Caldera magma body) presented by Brian Marshall at Summit 2000 Geological Society of America conference, or provide an independent model that explains elevated temperatures in the unsaturated zone from about 12 Ma to 2 Ma; and

B) In any analysis provided, address the effects of boundary conditions on the calculated results, and for the conductive cooling model, losses due to convection should be addressed; and

C) Support the Marshall model by additional data (U-Th-He with error bars to overlay the theoretical cooling curve or thermochronology fission track data and analysis), including data that constrain the time of peak temperature. Support Marshall model or any other model with data from analogous systems (i.e, are there younger calderas where temperature profiles in boreholes have been measured that would support conductive heating of the unsaturated zone for kilometers away from the eruption site); or

D) Complete the exclusion of the FEP by demonstrating that the consequences of hydrothermal activity on repository performance doesn't significantly affect the magnitude and time of the resulting expected annual dose.

E) In addition to items A, B, and C or D, DOE should address the timing and mode of formation of secondary mineralization for the Type B faults which record elevated temperatures (calcite twinning). Explain or interpret the apparent saturated conditions of mineralization in Class B faults. If DOE would like to argue that the twinning thickness is due to frictional heating and does not reflect temperature of fluids during formation, then DOE will need to provide a technical basis for their assertion.

The information provided below is reference information for documents that are cited in presentations given at the Evolution of the Near-Field Environment Technical Exchange but are not Analysis/Model Reports (AMRs) and Process Model Reports (PMRs). All citations and were reviewed to ensure that document numbers were included where appropriate (i.e., for AMRs and PMRs), but no additional information for AMRs and PMRs is provided here. The information was obtained from the Project Document Input Reference System, the Technical Information Center, and the Reference Information System.

Non-AMR and Non-PMR References for Sonnenthal and Apps Presentation on Coupled THC Processes Affecting the CHn

Broxton, D.E.; Bish, D.L.; and Warren, R.G. 1987. "Distribution and Chemistry of Diagenetic Minerals at Yucca Mountain, Nye County, Nevada." *Clays and Clay Minerals, 35,* (2), 89-110. Long Island City, New York: Pergamon Press. TIC: 203900. [102004] Listed on page 12

Carey, J.W. and Bish, D.L. 1996. "Equilibrium in the Clinoptilolite-H2O System." *American Mineralogist, 81,* 952-962. Washington, D.C.: Mineralogical Society of America. TIC: 233145. [105200] Listed on pages 15, 16, 17

Carey, J.W. and Bish, D.L. 1997. "Calorimetric Measurement of the Enthalpy of Hydration of Clinoptilolite." *Clays and Clay Minerals, 45,* (6), 826-833. [Long Island City, New York: Pergamon Press]. TIC: 235733. [128770] Listed on page 15, 17

Chipera, S.J. and Bish, D.L. 1997. "Equilibrium Modeling of Clinoptilolite-Analcime Equilibria at Yucca Mountain, Nevada." *Clays and Clay Minerals, 45,* (2), 226-239. Long Island City, New York: Pergamon Press. TIC: 233948. [105079] Listed on page 12

Dibble, W. E., Jr. and Tiller, W. A., 1981. Non-equilibrium water/rock interactions - I. Model for interface—controlled reactions. Geochimica et Cosmochimica Acta, vol. 45, p. 79-92. TIC: 240397. Listed on page 17

Dibble, W.E., Jr. and Tiller, W.A. 1981. "Kinetic Model of Zeolite Paragenesis in Tuffaceous Sediments." *Clays and Clay Minerals, 29,* (5), 323-329. [Long Island, New York: Pergamon Press]. TIC: 221129. [105386] Listed on pages 12, 16, 17

Duffy, C.J. 1993. *Kinetics of Silica-Phase Transitions.* LA-12564-MS. Los Alamos, New Mexico: Los Alamos National Laboratory. ACC: NNA.19900112.0346. [105481] Listed on page 13

Duffy, C.J. 1993. *Preliminary Conceptual Model for Mineral Evolution in Yucca Mountain.* LA-12708-MS. Los Alamos, New Mexico: Los Alamos National Laboratory. ACC: NNA.19900117.0152. [100740] Listed on pages 13, 16, 17

Note: Numbers in brackets [ ] are reference numbers for the DIR System.

Non-AMR and Non-PMR References for Hardin Presentation on Coupled Processes

Tsang, C-F. and Mangold, D.C., eds. 1984. *Panel Report on Coupled Thermo-Mechanical-Hydro-Chemical Processes Associated with a Nuclear Waste Repository.* LBL-18250. Berkeley, California: Lawrence Berkeley Laboratory. ACC: MOL.19981026.0041. [101058] Listed on page 14

Hardin, E.L. and Chesnut, D.A., 1997. *Synthesis Report on Thermally Driven Coupled Processes.* UCRL-ID-128495. Livermore, California: Lawrence Livermore National Laboratory. TIC: 234838. [150043] Listed on page 17

Non-AMR and Non-PMR References for Stockman Presentation on Thermal-Hydrological-Chemical Effects on Radionuclide Release

McCright, R.D. 1998. *Corrosion Data and Modeling, Update for Viability Assessment.* Volume 3 of *Engineered Materials Characterization Report.* UCRL-ID-119564, Rev. 1.1. Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19980806.0177. [114637] Cited on page 10; listed on page 23

Note: Numbers in brackets [ ] are reference numbers for the DIR System.

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

Evolution of The Near Field Environment

Presented to:
DOE/NRC Technical Exchange on Key Technical Issue and Subissues Related to Evolution of the Near-Field Environment

Presented by:
Deborah Barr
Yucca Mountain Site Characterization Office
Department of Energy

January 9-12, 2001
Pleasanton, CA

YUCCA MOUNTAIN PROJECT

Outline

- Purpose of the Technical Exchange
- Identification of Subissues
- Background
- Key DOE Activities Supporting Resolution of the Key Technical Issue
- Status of Subissue Acceptance Criteria from the Evolution of the Near-Field Environment Issue Resolution Status Report, Rev 03
- Status of NRC comments associated with Subissues

Purpose of Technical Exchange

- Present and agree on approach to close Subissues 1, 2, 3, and 4 and associated NRC comments for the Evolution of the Near-Field Environment Key Technical Issue
- Describe how evolution of the near-field environment is addressed in the Total System Performance Assessment
- Provide update on DOE's progress made with identifying and screening of features, events, and processes related to coupled-process models
- Provide update on DOE's progress made in enhancing coupled-process models and its test program
- Provide an overview of the treatment of model and data uncertainties

Current Subissues

- **Subissue 1:** Effects of Coupled Thermal-Hydrologic-Chemical Processes on Drift Seepage and Flow in the Unsaturated Zone
- **Subissue 2:** Effects of Coupled Thermal-Hydrologic-Chemical Processes on the Waste Package Chemical Environment
- **Subissue 3:** Effects of Coupled Thermal-Hydrologic-Chemical Processes on the Chemical Environment for Radionuclide Release

Current Subissues
(Continued)

- **Subissue 4:** Effects of Coupled Thermal-Hydrologic-Chemical Processes on Radionuclide Transport through Engineered and Natural Barriers
- **Subissue 5:** Effects of Coupled Thermal-Hydrologic-Chemical Processes on Potential Nuclear Criticality in the Near Field

Background

- **Subissue 5**
  - Addressed in a Key Technical Issue meeting in October 2000 and dispositioned as Closed-Pending
  - No additional discussion of this subissue is planned for this meeting
- **Acceptance criteria in the Evolution of the Near Field Issue Resolution Status Report, Rev 03 have changed significantly relative to acceptance criteria listed in Rev 02**
- **Lacking a specific cross-walk between the acceptance criteria in Rev 03 and those in Rev 02, DOE assumes that criteria in Rev 03 include any open items from Rev 02**

Background
(Continued)

- DOE's presentations address only the comments that have been provided by the NRC
- DOE understands that by addressing the items identified by the NRC as concerns, the acceptance criteria have been addressed sufficiently to discuss closure of the associated subissues

Key Activities Supporting Resolution of Evolution of the Near-Field Environment Issue

- Updated repository design to remove backfill
- Enhanced work scope to collect additional test data and validate coupled process models with test results
- Continuing work to quantify model and data uncertainties
- Revising Analysis Model Reports and Process Model Reports, as necessary, to reflect improvements in coupled-process modeling and testing to better understand coupled processes

Subissue Acceptance Criteria Status Subissues 1 through 4

Acceptance Criteria	NRC IRSR Rev. 3 Status	DOE Proposed Status
1) Integration for Evolution of the Near-Field Environment	Open	Closed-Pending
2) Data and Model Justification for Evolution of the Near-Field Environment	Open	Closed-Pending
3) Data Uncertainty for Evolution of the Near-Field Environment	Open	Closed-Pending
4) Model Uncertainty for Evolution of the Near-Field Environment	Open	Closed-Pending
5) Model Support for Evolution of the Near-Field Environment	Open	Closed-Pending

Note: Subissue 5 has been previously dispositioned in the October Technical Exchange on Criticality and will not be addressed at this meeting

NRC Comments About Effects of Coupled THC Process on Drift Seepage and Flow in the Unsaturated Zone

Comment	Addressed in Presentations
1) Alteration of Calico Hills Unit	Alteration of Calico Hills Unit
2) Interaction between Tuff Rock and cementitious materials in ventilation shafts and tunnels	Effects of Cementitious Materials
3) Mineral precipitation in fractures or at fracture/matrix interface	Mineral Precipitation
4) Software verification of TOUGHREACT	No presentation. Information provided to NRC
5) Inadequate screening arguments of Features, Events, and Processes	To be Addressed in TSPAI Technical Exchange

NRC Comments About Effects of Coupled THC Process on the Waste Package Chemical Environment

Comment	Addressed in Presentations
1) Define the near-field geochemical environment important to drip shield and waste package	In-drift Geochemical Environment
2) Technical bases for coupling, decoupling of thermal-hydrologic-chemical processes	Coupled-Processes and Model Integration
3) Technical assumption that processes can be treated separately without biasing water evolution predictions	Coupled-Processes and Model Integration
4) Technical justification for exclusion of hydrothermal activity Features, Events, and Processes	Features, Events, and Processes presented during Thermal Effects on Flow Key Technical Issue Meeting

NRC Comments About Effects of Coupled THC Process on the Waste Package Chemical Environment (Continued)

Comment	Addressed in Presentations
5) Provide information on water chemistry	Assumption of Chemical Equilibrium
6) Provide information on performance of Ti drip shield	Range of Water Chemistry and Trace Elements in Waste Package Chemical Environment
7) Technical bases that reaction proceed to equilibrium	Assumption of Chemical Equiliburium
8) Data uncertainties should be evaluated	Data Uncertainties and Sensitivity Studies
9) Use of alternative thermodynamic data does not capture intent of alternative criterion model	No presentation. NRC staff stated it considered comment resolved
10) Perform additional sensitivity studies to identifvy limitations of models	Data Uncertainties and Sensitivity Studies
11) Additional work needed to evaluate model limitation	No "Subissue 2" presentation

NRC Comments About Effects of Coupled THC Process on the Chemical Environment for Radionuclide Release

Comment	Addressed in Presentations
1) Abstraction of in-package chemistry ignores the potential effect of early stage high temp. phenomena	Thermal-Hydrological-Chemical Effects on Radionuclide Release
2) Abstraction of in-package chemistry ignores the potential interaction with grouted rock bolts	Thermal-Hydrological-Chemical Effects on Radionuclide Release
3) Abstraction of Commercial Spent Nuclear Fuel degradation ignores the potential effect of radiolytic production of acid	Thermal-Hydrological-Chemical Effects on Radionuclide Release
4) Provide a stronger technical basis for exclusion of irreversible attachment for Spent Nuclear Fuel colloids	Thermal-Hydrological-Chemical Effects on Radionuclide Release
5) State which radionuclides to be included in colloid attachment modeling. Provide technical basis for that list	Thermal-Hydrological-Chemical Effects on Radionuclide Release
6) Provide technical basis for limiting in-drift water chemistry for purposes of colloid modeling	Colloid Transport in the Unsaturated Zone

NRC Comments About Effects of Coupled THC Process on the Chemical Environment for Radionuclide Release (Continued)

Comment	Addressed in Presentations
7) Analysis Model Report on in-package chemistry does not provide enough information	Thermal-Hydrological-Chemical Effects on Radionuclide Release
8) Status on verification of input surface areas waste package dissol rates, thermo. database	Thermal-Hydrological-Chemical Effects on Radionuclide Release
9) (Duplicate of Number 8)	Thermal-Hydrological-Chemical Effects on Radionuclide Release
10) In-package chemistry Analysis Model Report abstraction does not explain good fit the response surfaces are to values computed using EQ/6	Thermal-Hydrological-Chemical Effects on Radionuclide Release
11) DOE needs to conduct a sensitivity analysis to determine if temperature effects are important	Thermal-Hydrological-Chemical Effects on Radionuclide Release

NRC Comments About Effects of Coupled THC Process on the Chemical Environment for Radionuclide Release (Continued)

Comment	Addressed in Presentations
12) Provide reasonable assurance that the adopted maximum concentration of irreversibly-attached Pu is bounding	Thermal-Hydrological-Chemical Effects on Radionuclide Release
13) DOE needs to provide a better technical justification for not using the more conservative approach of minimum ionic strength	Thermal-Hydrological-Chemical Effects on Radionuclide Release
14) DOE needs to provide a technical bases for the corrosion rates used in their calculations	Thermal-Hydrological-Chemical Effects on Radionuclide Release
15) DOE should evaluate the performance of the alternative colloid release model	Thermal-Hydrological-Chemical Effects on Radionuclide Release
16) No alternative models for in-drift colloid transport are discussed	Thermal-Hydrological-Chemical Effects on Radionuclide Release
17) Analysis assumes water may circulate freely enough in partially degraded waste package	Thermal-Hydrological-Chemical Effects on Radionuclide Release
18) In-waste package Analysis Model Report states that it's not possible to fully validate the model. DOE should identify steps that will be conducted to validate the models	Thermal-Hydrological-Chemical Effects on Radionuclide Release
19) DOE predictions of in-package chemistry based on the EQ3/6 code have not been verified by emperical observations	Thermal-Hydrological-Chemical Effects on Radionuclide Release

NRC Comments About Effects of Coupled THC Process on Radionuclide Transport Through the Engineered and Natural Barriers

Comment	Addressed in Presentations
1) Provide additional technical bases for exclusion of 21 Features, Events, and Processes	No presentation. This will be addressed at the TSPAI Technical Exchange
2) Provide qualified version of TOUGHREACT software source code	No presentation. DOE will provide the executable source code to NRC
3) Provide consistent explanations that thermal-hydrological-chemical processes from the repository will not adversely affect the properties of the natural barrier using 70° C	Coupled thermal-Hydrological-Chemical Processes Affecting the Calico Hills Hydrogeological Unit
4) Provide information on the retardation coefficients (k_ds) and matrix diffusion obtained under anticipated thermal-hydrological-chemical conditions	No presentation. NRC staff stated it considered commend resolved
5) Provide data supporting its current conceptual approach for colloid transport in the unsaturated zone	Colloidal Transport in the Unsaturated Zone
6) Calculational error reflected in Engineered Barrier System Process Model Report	No presentation. Error was corrected, correction was forwarded to NRC on 12/12/00
7) Data file could not be accessed through the Internet-based technical data management system. Data should be made available	No presentation. Data tracking number was provided to NRC on 12/22/00

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

NRC Comments Related to Total System Performance Assessment Treatment of Engineered Barrier System Chemical Environments

Presented to:
DOE-NRC Technical Exchange on Key Technical Issue and Subissues Related to Evolution of the Near-Field Environment

Presented by:
James Nowak
Civilian Radioactive Waste Management System
Management and Operating Contractor

January 9-12, 2001
Pleasanton, CA

YUCCA MOUNTAIN PROJECT

Outline

- **Presentation Objectives**
- **For NRC comments on Total System Performance Assessment treatment of Engineered Barrier System chemical environments associated with the Evolution of the Near-Field Environment Key Technical Issue, this presentation will**
  - Describe the Total System Performance Assessment treatment of Engineered Barrier System chemical environments
  - Discuss the technical basis for resolution of NRC comments related to Total System Performance Assessment
- **Conclusions**

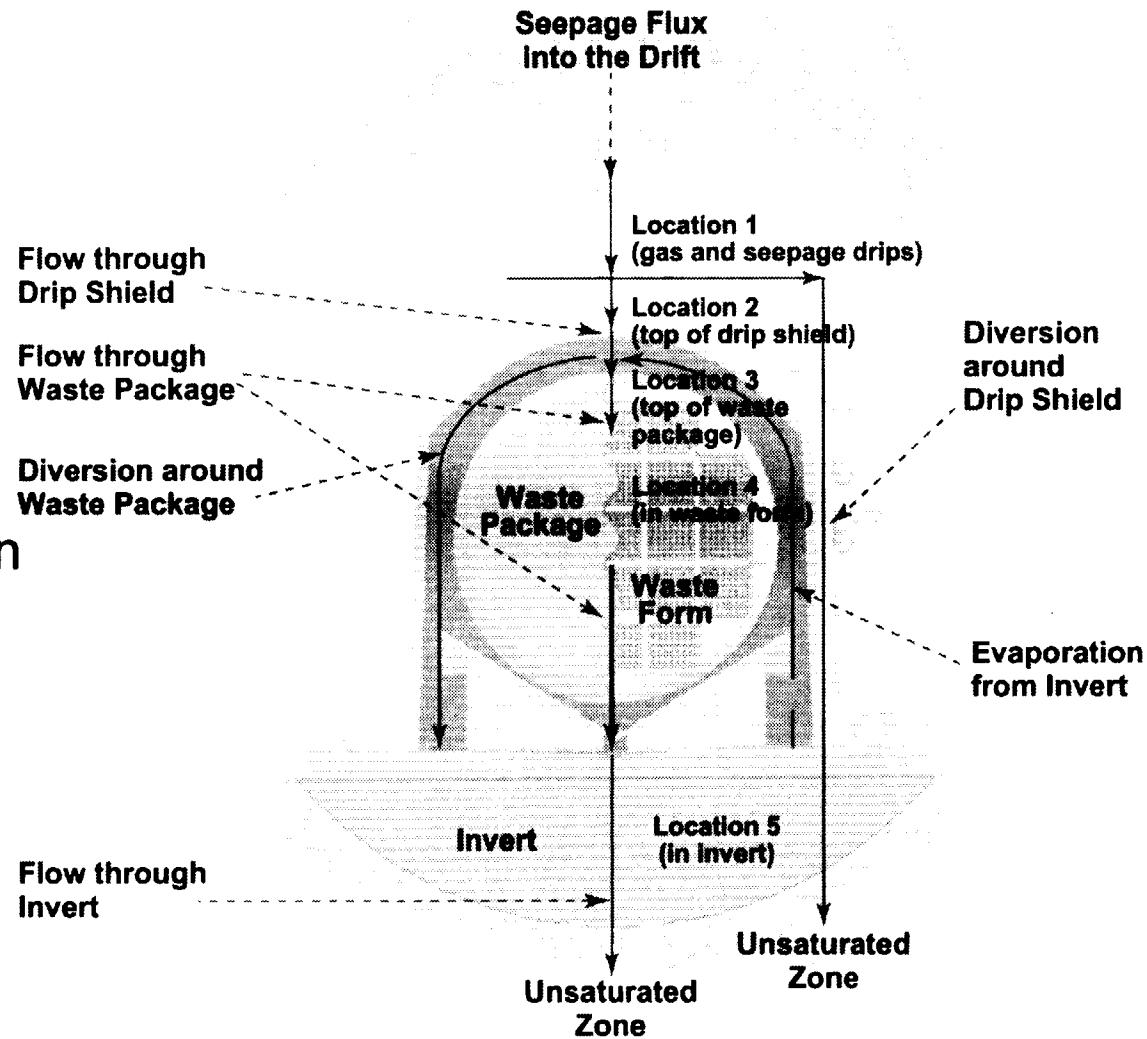
Presentation Objectives

- **Describe the Total System Performance Assessment treatment of Engineered Barrier System chemical environments**
- **Describe the Total System Performance Assessment treatment of the subjects of NRC comments related to the subissues of the Evolution of the Near-Field Environment Key Technical Issue**
- **DOE has determined**
  - Conclusions from the physical and chemical environment abstraction models are valid for the coupled system, and appropriate water compositions have been used
  - The current Total System Performance Assessment model for invert water chemistry for the purpose of colloid modeling is adequate and conservative
  - Exclusion of appropriate alternative models for in-drift colloid transport is appropriate and conservative

Total System Performance Assessment Context of Engineered Barrier System Chemical Environments

Local chemical environments captured at critical locations along transport paths:

- On waste package
- In waste form - discussed in the following presentation
- In invert
- Transport path is discussed in the second presentation following this one



Reference: TDR-WIS-PA-000001 Rev 00 ICN01, Figure 3.3-13

Total System Performance Assessment Context of Engineered Barrier System Chemical Environments (Continued)

In-drift Thermal-Hydrologic, Seepage, and Thermal-Hydrologic-Chemical Abstraction Inputs

- Temperature - local
- Relative humidity - local
- Water evaporation rates - local
- Incoming seepage rate and composition - drift wall
- Incoming gas composition - drift wall

Total System Performance Assessment Context of Engineered Barrier System Chemical Environments (Continued)

Drift Wall Seepage Water and Gas Composition

- **Water and gas chemistry abstractions are from the drift-scale thermal-hydrologic-chemical seepage model at the drift wall**
  - Total System Performance Assessment abstractions are from results for a thermally evolving system
  - Uncertainty in infiltration rate has been considered

Total System Performance Assessment Context of Engineered Barrier System Chemical Environments (Continued)

Drift Wall Seepage Water and Gas Composition (Continued)

- Four time periods were applied as a boundary condition for Engineered Barrier System chemical environments abstracted models - table based on mean infiltration case

Adapted from MDL-NBS-HS-000001 Rev 00

Aqueous Species	Gaseous Species	Minerals	
Both models:	Both models:	Both models:	
H^+	CO_2	Calcite	Amorphous Silica
Ca^{+2}		Tridymite	Gypsum
Na^+		α–Cristobalite	Glass
H_2O		Quartz	
SiO_2		Complex model only:	
Cl^-		Hematite	K-Smectite
HCO_3^-		Fluorite	Illite
SO_4^{-2}		Goethite	Kaolinite
Complex model only:		Albite	Sepiolite
Mg^{+2}		Microcline	Stellerite
K^+		Anorthite	Heulandite
AlO_2^-		Ca-Smectite	Mordenite
$HFeO_2$		Mg-Smectite	Clinoptilolite
F^-		Na-Smectite	

Source: CRWMS M&O (2000, U0110, Tables 7, 8)

Adapted from ANL-NBS-HS-000029 Rev 00

Period	Period 1: Preclosure	Period 2: Boiling	Period 3: Transitional Cool Down	Period 4: Extended Cool Down
Time	0–50 years	50–1,000 years	1,000–2,000 years	2,000+ years
Constituents from simplified THC model				
CO_2, log vol. frac.	–2.8	–6.5	–3.0	–2.0
pH	8.2	8.1	7.8	7.3
Ca^{+2}, molal	1.7×10^{-3}	6.4×10^{-4}	1.0×10^{-3}	1.8×10^{-3}
Na^+, molal	3.0×10^{-3}	1.4×10^{-3}	2.6×10^{-3}	2.6×10^{-3}
SiO_2, molal	1.5×10^{-3}	1.5×10^{-3}	2.1×10^{-3}	1.2×10^{-3}
Cl^-, molal	3.7×10^{-3}	1.8×10^{-3}	3.2×10^{-3}	3.3×10^{-3}
HCO_3^-, molal	1.3×10^{-3}	1.9×10^{-4}	3.0×10^{-4}	2.1×10^{-3}
SO_4^{-2}, molal	1.3×10^{-3}	6.6×10^{-4}	1.2×10^{-3}	1.2×10^{-3}
Additional constituents from complex THC model				
Mg^{+2}, molal	4.0×10^{-6}	3.2×10^{-7}	1.6×10^{-6}	7.8×10^{-6}
K^+, molal	5.5×10^{-5}	8.5×10^{-5}	3.1×10^{-4}	1.0×10^{-4}
AlO_2^-, molal	1.0×10^{-10}	2.7×10^{-7}	6.8×10^{-8}	2.0×10^{-9}
$HFeO_2$, molal	1.1×10^{-10}	7.9×10^{-10}	4.1×10^{-10}	2.4×10^{11}
F^-, molal	5.0×10^{-5}	2.5×10^{-5}	4.5×10^{-5}	4.5×10^{-5}

Period 2 water chemistry represents condensate water that could potentially flow through a fracture to the drift wall

Total System Performance Assessment Context of Engineered Barrier System Chemical Environments (Continued)

Drift Wall Seepage Water and Gas Composition (Continued)

- **Propagation of hydrologic property set uncertainty through model abstractions**
  - *Low* and *high* infiltration flux water and gas compositions were compared and typically found to be less than an order of magnitude different (from the mean flux case) - in virtually all cases < 2x
- **Treatment of conceptual model uncertainty in model abstractions**
  - Flow Uncertainty - Drift-scale thermal-hydrologic-chemical seepage process model and subsequent abstractions are based on the dual permeability active fracture model
    - Basis: Thermal Test temperature results from Large Block Test, Single Heater Test, Drift Scale Heater Test
  - Geochemical System Uncertainty - Two mineral systems were used
    - Basis: Thermal Test chemistry results from Drift Scale Heater Test

Total System Performance Assessment Context of Engineered Barrier System Chemical Environments (Continued)

Drift Wall Seepage Water and Gas Composition (Continued)

- **References**
  - Drift-Scale Coupled Processes (DST and THC Seepage) Models (MDL-NBS-HS-000001 Rev 01, is in review)
  - Abstraction of Drift-Scale Coupled Processes (ANL-NBS-HS-000029 Rev 00)

NRC Total System Performance Assessment-Related Comments Associated with Subissue 2

- **NRC Comment**
  - A technical basis is required for the DOE assumption that processes, such as those described in the Gas Flux and Fugacity, Cementitious Materials, Microbial Effects, Corrosion Products, and Precipitates/Salts models can be treated separately without biasing predictions of how water composition will evolve over time in a complex natural and engineering environment subjected to a range of processes. This concern includes
    - Insufficient integration between the DOE's various physical and chemical environment models (i.e., the relationship between the water compositions used as inputs and outputs in the different process-level models)
    - The use of J-13 as an initial water composition

DOE Assumption that Processes Can Be Treated Separately

- **Basis for Resolution**
  - DOE response from a more general process model perspective will be presented by Ernest Hardin
  - All Engineered Barrier System chemical environment abstraction models include significant couplings with other models, and conclusions from each model are valid for the coupled system
  - Gas flux and composition - Explicitly coupled with thermal-hydrologic-chemical abstraction models. Coupling with microbial activity is being included
    - Sources and sinks for carbon dioxide and oxygen in relevant in-drift processes have been taken into account in current analysis/model reports. Additional evaluation of microbial source for carbon dioxide is underway

DOE Assumption that Processes Can Be Treated Separately (Continued)

- **Basis for Resolution (Continued)**
  - Precipitates/Salts - Explicitly integrated with thermal-hydrologic, thermal-hydrologic-chemical, seepage, and gas environment composition abstraction models
    - Use inputs of abstracted seepage rates, seepage compositions, CO_2 in gas, local in-drift evaporation rates, local relative humidities, and local temperatures
    - Take initial water composition from thermal-hydrologic-chemical seepage abstraction. J-13 water composition is not used

DOE Assumption that Processes Can Be Treated Separately (Continued)

- **Basis for Resolution (Continued)**
  - Microbial effects - Model predicts upper bound on microbial mass for conditions due to effects of all other relevant processes
    - Nutrients include all major components of all Engineered Barrier System materials and degradation products
    - Microbes viable below 120° C in virtually any chemical environment containing sufficient nutrients and redox energy
    - Microbially generated carbon dioxide is now being evaluated
  - Cementitious materials in Engineered Barrier System (cementitious grouts) - Potential sources and sinks for carbon dioxide in relevant processes have been taken into account. Coupling with seepage has been included. Current analysis/model reports show effect to be negligible
  - Corrosion products
    - Coupling of corrosion reactions with other processes is retained
  - Waste package contents are discussed later in this presentation

DOE Assumption that Processes Can Be Treated Separately (Continued)

- **References**
  - Abstraction of Drift-Scale Coupled Processes (ANL-NBS-HS-000029 Rev 00)
  - Abstraction of NFE Drift Thermodynamic Environment and Percolation Flux (ANL-EBS-HS-000003 Rev 00)
  - Engineered Barrier System Physical and Chemical Environment Model (ANL-EBS-MD-000033 Rev 01)
  - In-Drift Corrosion Products (ANL-EBS-MD-000041 Rev 00)
  - In-Drift Microbial Communities (ANL-EBS-MD-000038 Rev 00)
  - In-Drift Precipitates/Salts Analysis (ANL-EBS-MD-000045 Rev 00)
  - Physical and Chemical Environmental Abstraction Model (ANL-EBS-MD-000046 Rev 00 ICN 01)
  - Precipitates/Salts Model Results for THC Abstraction (CAL-EB-PA-000008 Rev 00)

Conclusions

- All physical and chemical environment abstraction models include significant couplings with other models, and conclusions from each model are valid for the coupled system
- From the reported data and models and the ongoing work, sufficient information will be available to assure that there is sufficient integration/coupling among Engineered Barrier System chemical models and that appropriate water compositions have been used
- DOE considers that the NRC comment on modeled treatment of processes discussed in this presentation has been addressed. The information presented and planned studies to confirm expectations about microbially generated carbon dioxide and colloids support a status of Closed-Pending for Subissue 2

NRC Total System Performance Assessment-Related Comments Associated with Subissue 4

- **NRC Comment**
  - … DOE should provide a technical basis for limiting in-drift water chemistry (for purposes of colloid modeling) to either waste package water or a mixture of waste package water and J-13

Limiting In-Drift Water Chemistry

- **Basis for Resolution**
  - The current Total System Performance Assessment model for invert water chemistry is conservative
    - Colloidal radionuclides arriving in the invert by advection and diffusion (if advection does not dominate) pass unretarded through to the unsaturated zone by the same transport mechanism(s)
    - Invert water chemistry calculated from Precipitates/Salts abstraction is used to determine an upper stability limit for the colloidal radionuclide concentrations in the invert
    - The flux of colloidal radionuclides to the unsaturated zone would be smaller than the flux coming from the waste package *if* the upper stability limit were exceeded when colloids from the waste package were mixed with water in the invert
    - Colloidal radionuclide fluxes from the invert to the unsaturated zone and from the waste package are the same in virtually every realization in Total System Performance Assessment calculations. Therefore, invert water chemistry, as modeled, does not reduce colloidal radionuclide releases

Limiting In-Drift Water Chemistry
(Continued)

- **References**
  - EBS Radionuclide Transport Abstraction (ANL-WIS-PA-00000 Rev 00 ICN 02)
  - In-Drift Colloids and Concentration (ANL-EBS-MD-000042 Rev 00)

Conclusions

- The current Total System Performance Assessment model for invert water chemistry models colloids conservatively
- Calculated radionuclide release fluxes from the invert show that invert water chemistry as modeled does not reduce colloidal radionuclide releases to the unsaturated zone
- Reported models and results are available to support the conservatism of the invert water chemistry approach

Conclusions
(Continued)

- DOE considers the NRC comments on invert water chemistry discussed in this presentation have been addressed and that this information supports a status of Closed-Pending for Subissue 4

NRC Total System Performance Assessment-Related Comments Associated with Subissue 3

- **NRC Comments**
  - The DOE should provide a technical basis for limiting in-drift water chemistry for purposes of colloid modeling to either waste package water or a mixture of waste package water and J-13
  - No alternative models for in-drift colloid transport are discussed. The alternative model presented in the waste form colloid release abstraction is not appropriate for in-drift transport

Technical Basis for Limiting In-Drift Water Chemistry for Purposes of Colloid Modeling

- **Basis for Resolution**
  - This comment has been addressed. Refer to the response to the NRC comment related to Subissue 4
- **Reference**
  - Engineered Barrier System Radionucldie Transport Abstraction (ANL-WIS-PA-000001 Rev 00 ICN 02)

Alternative Models for In-Drift Colloid Transport

- **NRC Comment**
  - No alternative models for in-drift colloid transport are discussed. The alternative model presented in the waste form colloid release abstraction is not appropriate for in-drift transport
- **Basis for Resolution**
  - Exclusion of appropriate alternative model components for in-drift colloid transport is conservative
    - Filtration – traps colloids so that the concentration of colloids is reduced
    - Lateral diffusion/dispersion – spreads the release
  - These processes tend to reduce and delay radionuclide releases

Alternative Models for In-Drift Colloid Transport (Continued)

- **Reference**
  - Engineered Barrier System Radionuclide Transport Abstraction (ANL-WIS-PA-000001 Rev 00 ICN 02)
- **Conclusions**
  - The current Total System Performance Assessment model for invert water chemistry for the purpose of colloid modeling is conservative
  - Exclusion of appropriate alternative model components for in-drift colloid transport is conservative
  - DOE has appropriately considered credible alternative models for in-drift colloid transport
  - DOE considers the NRC comment on alternative models for in-drift water colloid transport discussed in this presentation has been addressed and this information supports a status of Closed-Pending for Subissue 3

Overall Conclusions

- The physical and chemical environment abstraction models include significant couplings with other models, and conclusions from each model are valid for the coupled system
- The current Total System Performance Assessment model for invert water chemistry models colloids conservatively, and it has no effect on release to the unsaturated zone. Different water compositions could decrease release but would not increase release
- Exclusion of appropriate alternative models for in-drift colloid transport is also conservative. Potential alternative models would make the model less conservative

Overall Conclusions
(Continued)

- DOE considers that the NRC comments related to the Total System Performance Assessment Treatment of Engineered Barrier System Chemical Environments have been addressed. The information presented and the planned study to confirm expectations about the importance of microbially generated carbon dioxide and colloids support a status of Closed-Pending for Subissues 2, 3, and 4

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

Subissue 3: NRC Comments Related to Total System Performance Assessment for the Site Recommendation Results Related to Waste Form Degradation

Presented to:
DOE-NRC Technical Exchange on Key Technical Issue and Subissues Related to Evolution of the Near-Field Environment

Presented by:
Rob Rechard
Civilian Radioactive Waste Management System Management and Operating Contractor

January 9-12, 2001
Pleasanton, CA

YUCCA MOUNTAIN PROJECT

Outline

- **Presentation Objectives**
- **Current Subissue Status**
- **Overall Total System Performance Assessment for the Site Recommendation Results**
- **Assumptions and intermediate results from two Waste Form Degradation Model components**
  - In-package chemistry
  - Colloidal concentration
- **Technical basis for Total System Performance Assessment**
  - Exclusion of geochemical, radiolytic, and coupled thermal-hydrological-chemical effects other than pH and ionic strength
  - Colloidal formation and transport
- **Conclusions**

Presentation Objectives

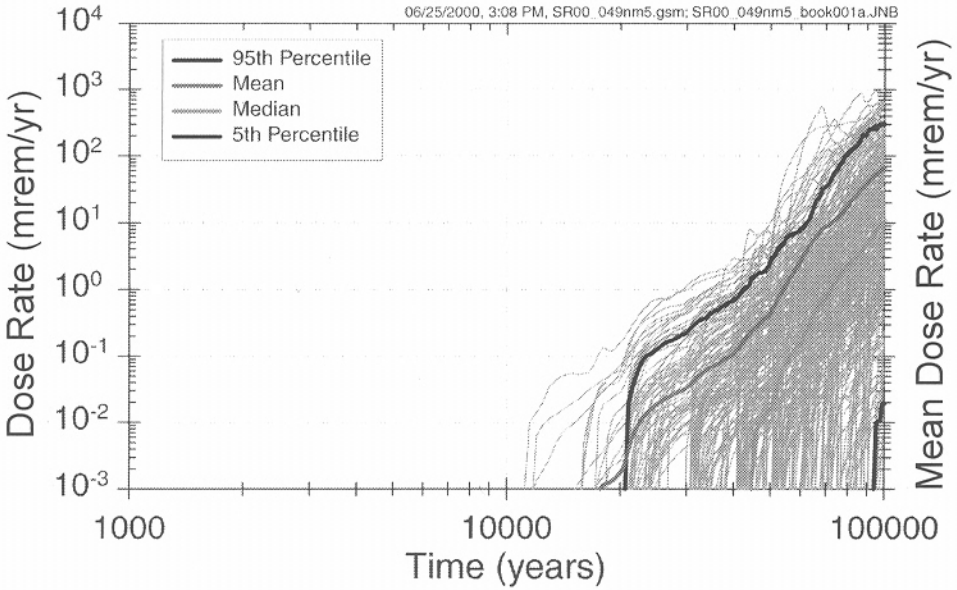
- Identify the main contributors to dose
- Present assumptions and results from Waste Form Degradation Model of Total System Performance Assessment for Site Recommendation to provide context for NRC comments related to Subissue 3 (thermal-hydrological-chemical effects on radionuclide release) of the Evolution of the Near-Field Environment Key Technical Issue
- Describe the basis for resolving NRC comments on colloidal formation and transport in the waste package for Subissue 3

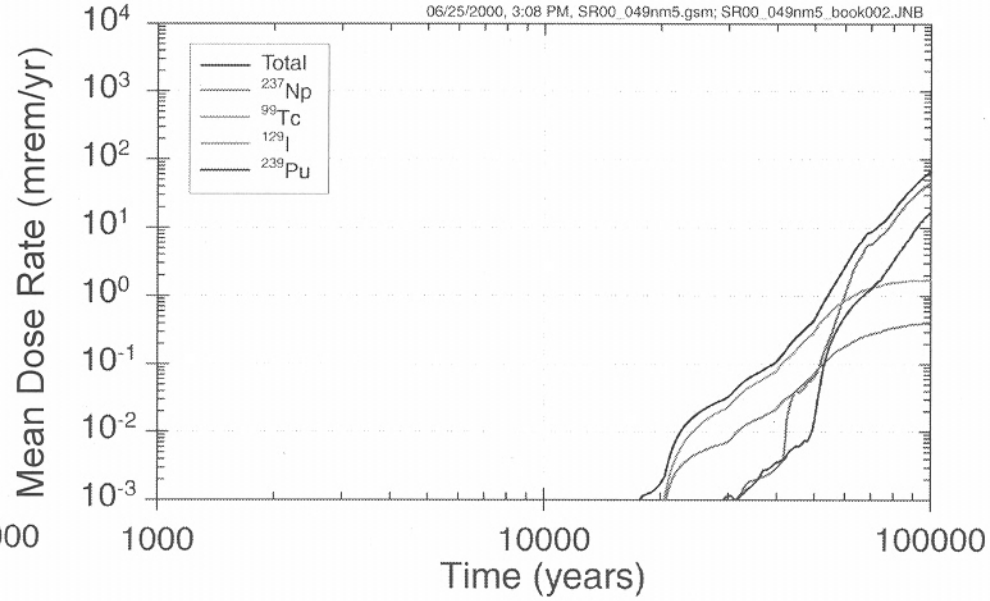
Current Subissue Status

- **Evolution of the Near-Field Environment Issue Resolution Status Report, Rev 03, indicates Subissue 3 is OPEN**

Main Contributors to Mean Dose

^{99}Tc and ^{237}Np contribute most to mean dose



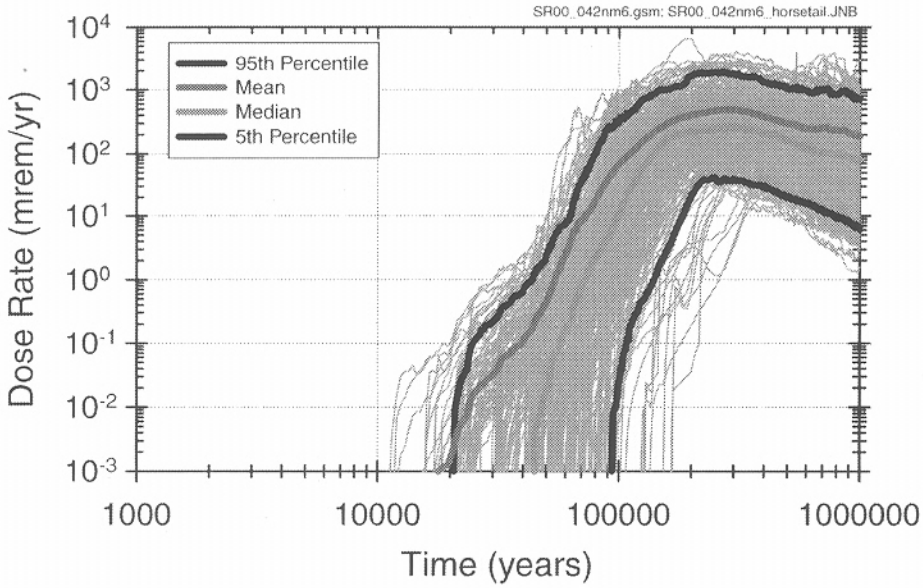


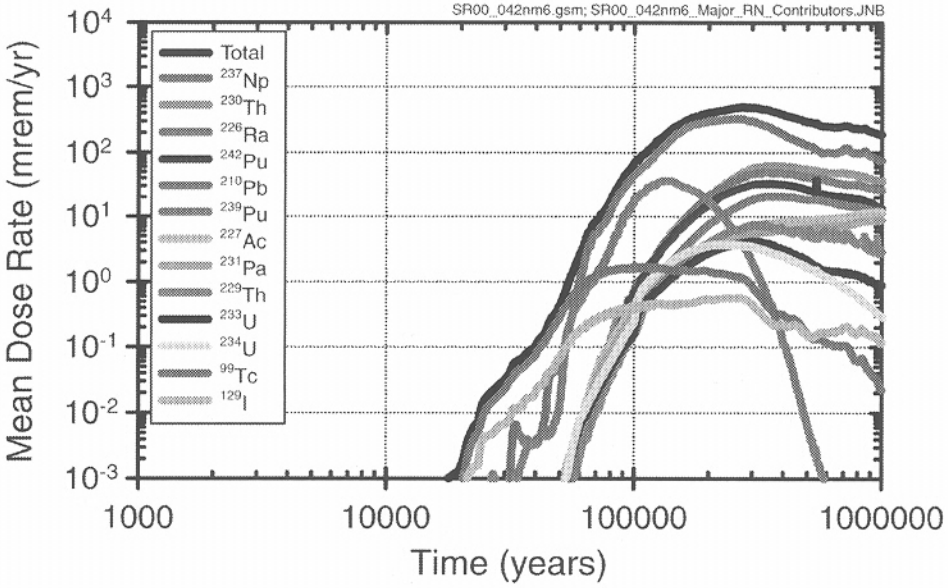
Reference: *Total System Performance Assessment for Site Recommendation,* TDR-WIS-PA-000001 REV 00 ICN 01, Figure 4.1-5

C01

Main Contributor to Peak Dose at 270,000 years

Peak Dose at 270,000 years is primarily from ^{237}Np



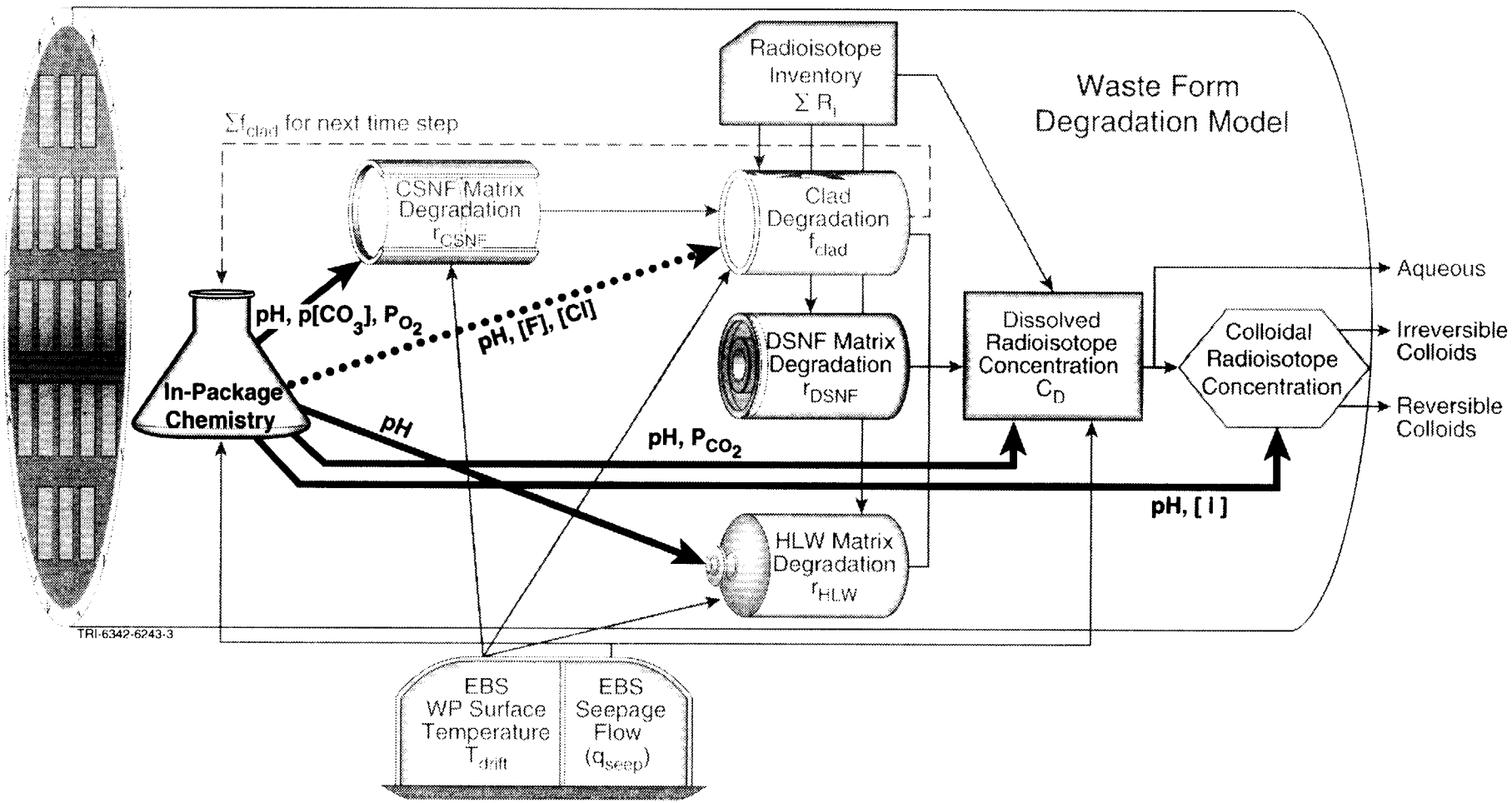


Reference: *Total System Performance Assessment for Site Recommendation,* TDR-WIS-PA-000001 REV 00 ICN 01, Figure 6.1-8

C02

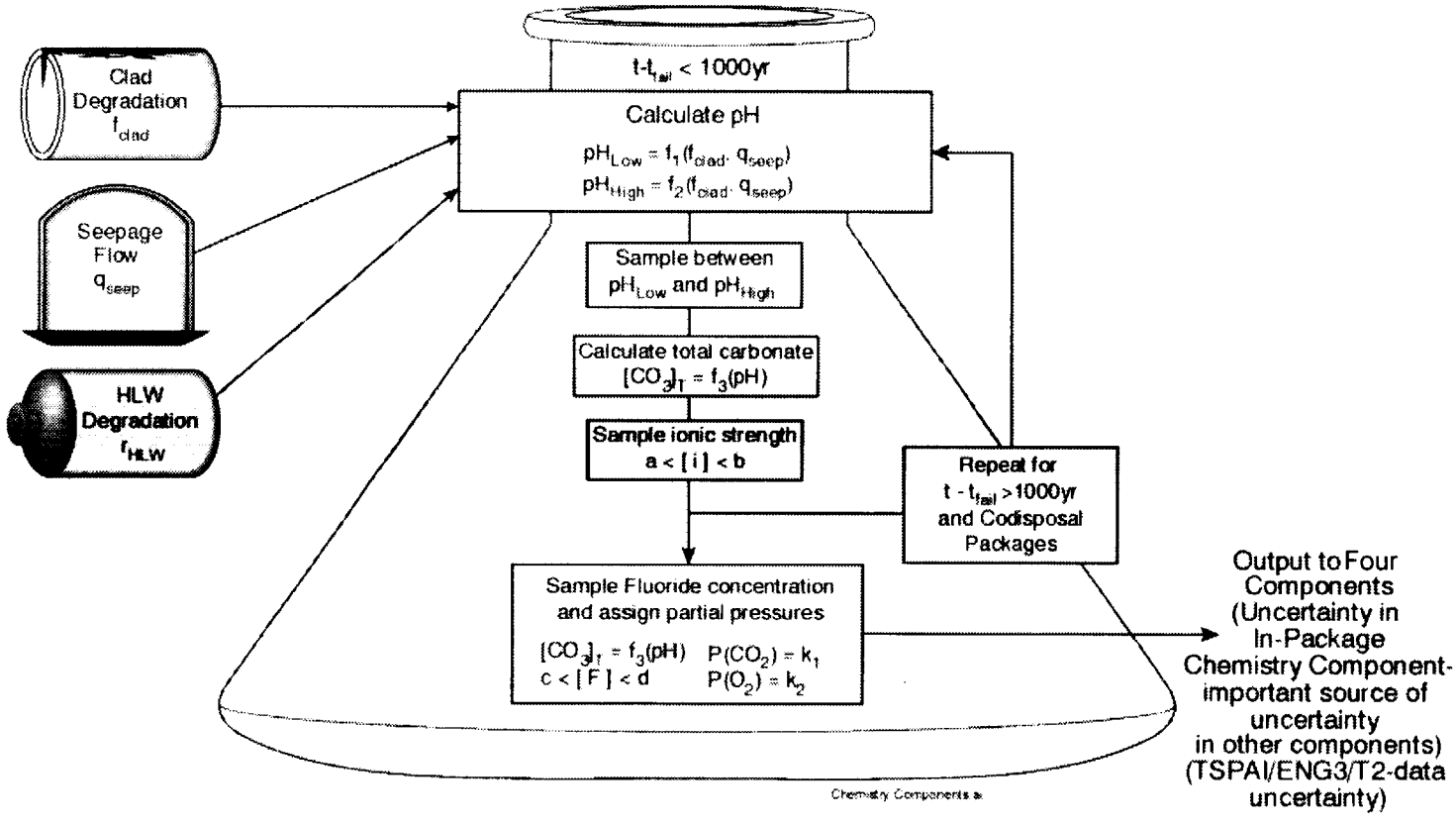
In-Package Chemistry Component Couples to Four Other Components

- **Addresses thermal-hydrological-chemical coupling issue in Subissue 3**
- **Uncertainty in chemistry contributes to uncertainty in four other components**



Reference: *Waste Form Degradation PMR*, TDR-WIS-MD-000001, Figure 1.5-3

In-Package Chemistry Component Assigns pH, $[CO_3]_T$, [i], [F], CO_2, and O_2



Reference: *Waste Form Degradation PMR*, TDR-WIS-MD-000001, Figure 3.2-2

Assumptions of In-Package Chemistry Component

- **Cladding, high-level waste, and basket (e.g., stainless steel) degradation rates, and fixed gas pressures (CO_2 and O_2) control chemistry**
  - Degradation rates of basket and High Level Waste reevaluated in revision to *Summary of In-Package Chemistry Analysis/Model Report*
- **Bulk chemistry approximated by well mixed, always oxidizing, full bathtub scenario at 25° C**
  - Localized chemistry (e.g., radiolysis) not included thus Cladding Degradation Component did not use [Cl] and [F]
  - Radiolysis discussed as feature, event, or process

References: *Waste Form Degradation PMR*, TDR-WIS-MD-000001, *Summary of In-Package Chemistry AMR*, ANL-EBS-MD-000050, and *Miscellaneous Waste Form FEPs, ANL-WIS-MD-000009*

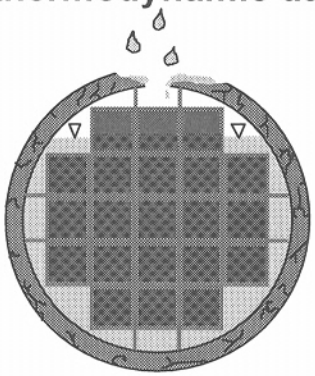
Assumptions of In-Package Chemistry Component
(Continued)

- **Chemical condition in waste package dominates; thus, J-13 well water can be used**
  - Influence of evaporation evaluated in revision of analysis model report
  - Influence of cement evaluated as feature, event, or process

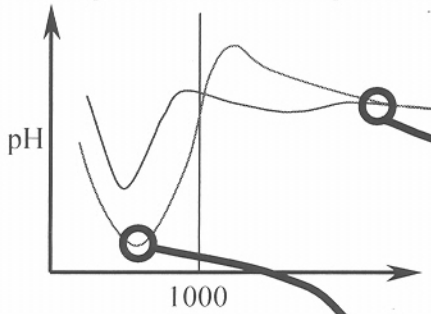
References: *Waste Form Degradation PMR*, TDR-WIS-MD-000001, *Summary of In-Package Chemistry AMR*, ANL-EBS-MD-000050, and *Miscellaneous Waste Form FEPs, ANL-WIS-MD-000009*

In-Package Chemistry Component Developed from Regression Analysis on EQ3/6 Runs

- Regression fit re-evaluated in revision to *In-Package Chemistry Abstraction Analysis/Model Report*
- Chemistry for pH in commercial spent nuclear fuel discretized into four segments in analysis/model report revision (with breaks at $2x10^2$,10^4,and $3x10^4$)
- Qualified thermodynamic data used in analysis/model report revision

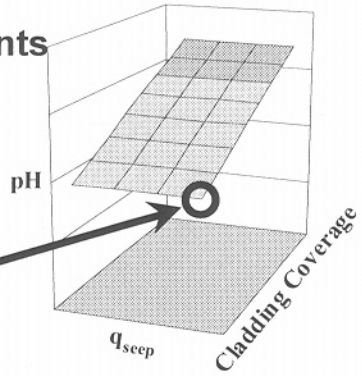


CSNF Conceptual Model

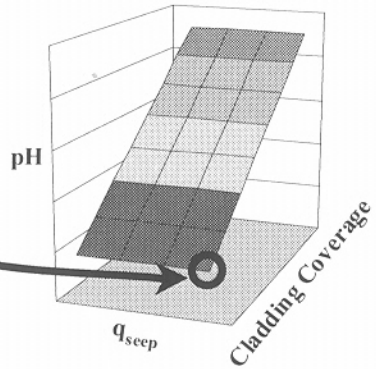


EQ3/6 Runs Varying:

- q_{seep}
- r_{steel}*
- r_{hlw}
- f_{clad}



pH Abstraction for > 1,000 Years



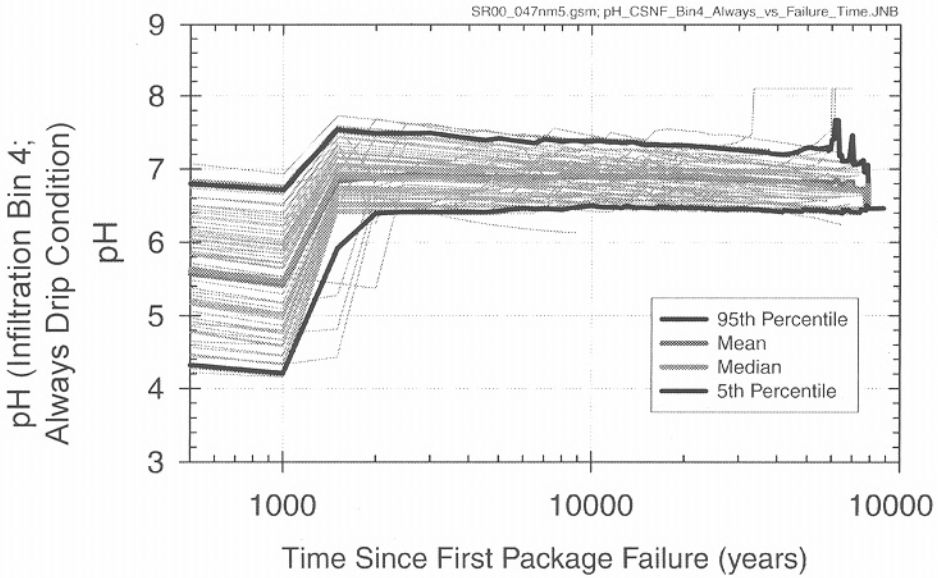
pH Abstraction for < 1000 Years

* Corrosion of steel releases sulfur, which can lower pH.
Reference: *In-Package Chemistry Abstraction AMR*, ANL-WIS-MD-000037

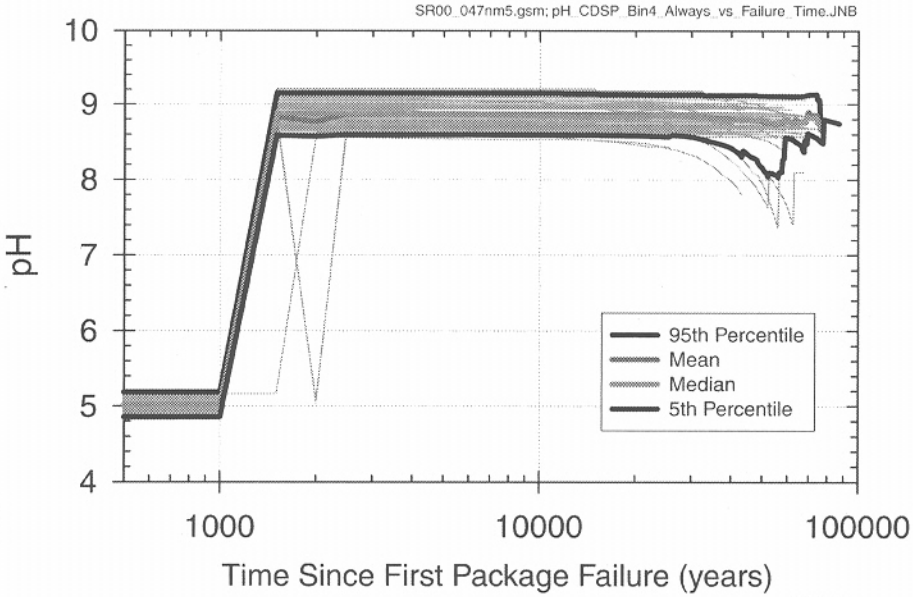
C03

Limited pH Uncertainty until Water Flows into Waste Package

Commercial Spent Nuclear Fuel



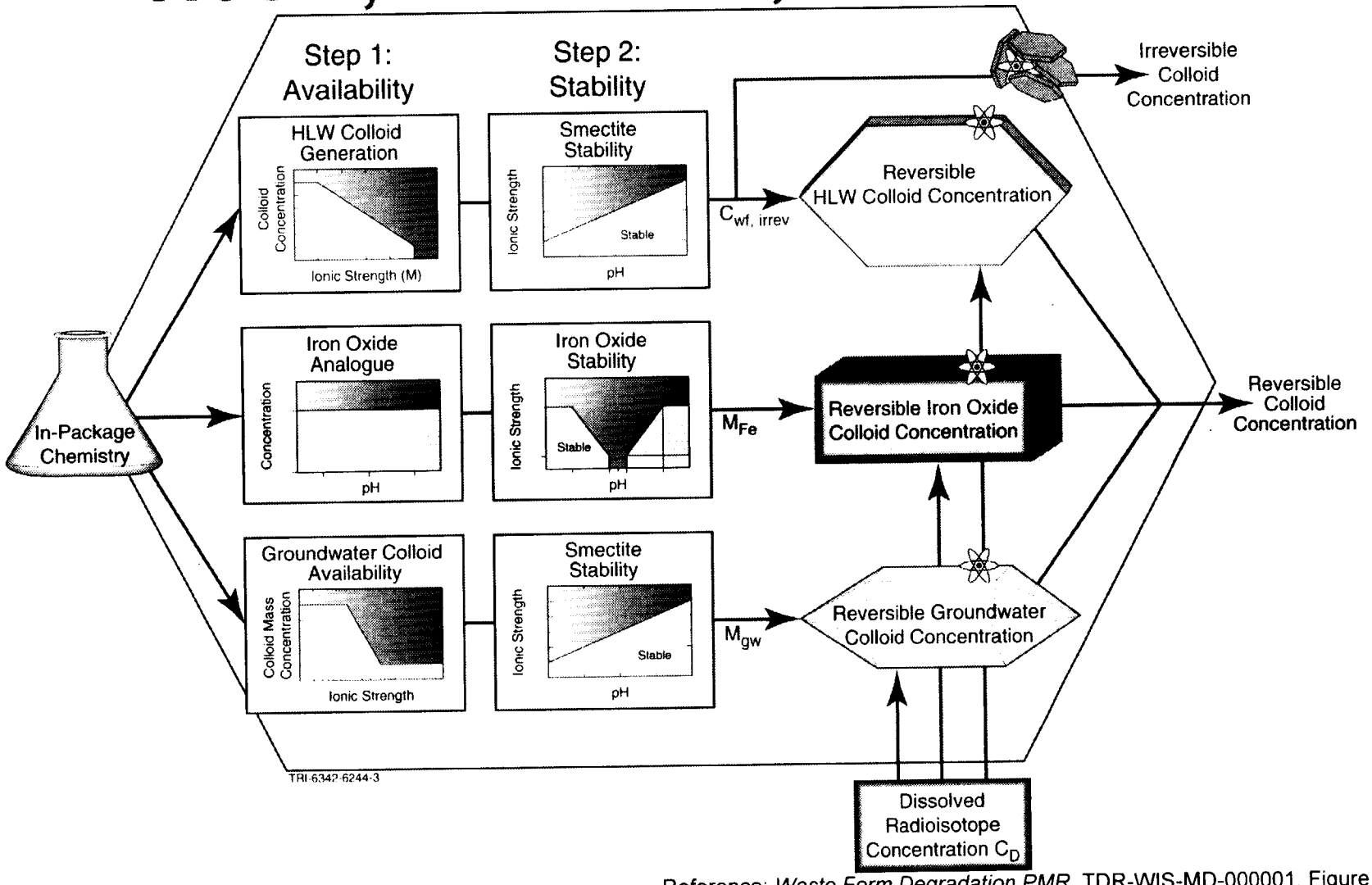
Co-Disposal



Reference: *Total System Performance Assessment for Site Recommendation*, TDR-WIS-PA-000001, Figure 3.5-8

C04

Colloidal Component Evaluates the Colloid Concentration on Three Types of Colloids: Waste, Iron Oxide, and Natural



Reference: *Waste Form Degradation PMR*, TDR-WIS-MD-000001, Figure 3.8-2

Assumptions for Colloid Component

- **Irreversible waste colloids from High-Level Waste only**
  - Tests on high-level waste determine maximum concentration of Pu colloids (and by analogy Am colloids)
  - Preliminary tests on commercial spent nuclear fuel show few colloids and no irreversible colloids (confirmatory tests are ongoing)
  - Only Pu and Am transported as *irreversible* colloids
- **Reversible colloids formed by iron oxides, all waste forms, and groundwater**
  - Interaction between colloid forms conservatively neglected
  - Pu, Am, Th (Ra, Pb), Pa (Ac) transported as *reversible* colloids

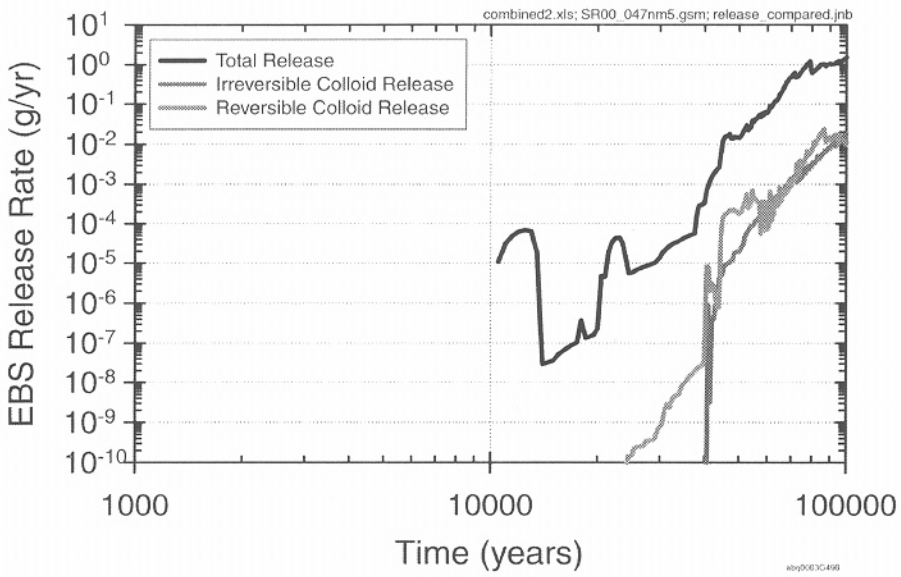
References: *Waste Form Degradation PMR*, TDR-WIS-MD-000001, and *Waste Form Colloid-Associated Concentration Limits: Abstraction and Summary AMR*, ANL-WIS-MD-000012

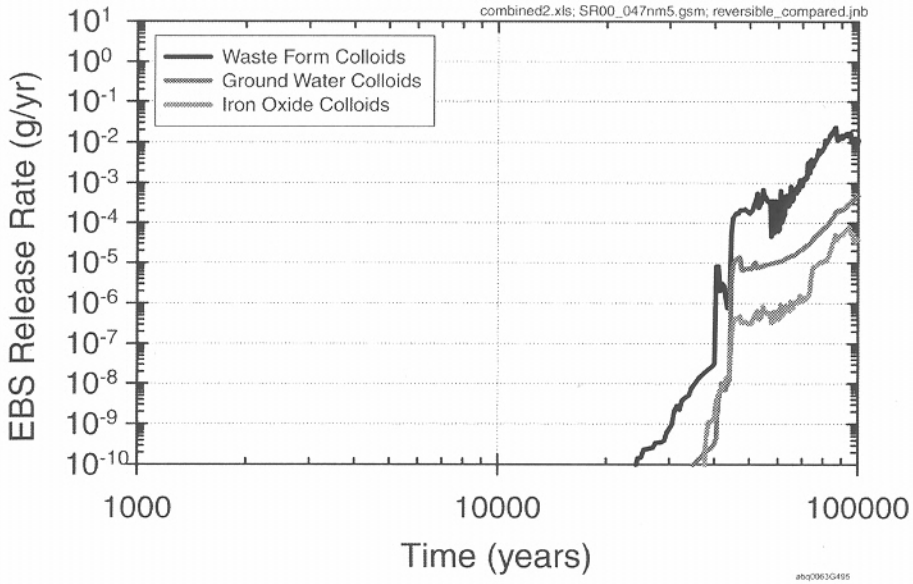
Assumptions for Colloid Component
(Continued)

- **Ionic strength and pH determine availability and stability**
  - Other effects cause colloid instability
- **No filtration or sorption within package**
- **Diffusion coefficient for colloids conservative**
  - Only 100 times less than aqueous diffusion
- **Colloids produced by microbes screened out**
  - Microbial colloids flocculate easily and thus are easily filtrated by porous material

References: *Waste Form Degradation PMR*, TDR-WIS-MD-000001, and *Waste Form Colloid-Associated Concentration Limits: Abstraction and Summary AMR*, ANL-WIS-MD-000012

Colloids Contribute Only a Small Fraction to Release of ^{239}Pu





Container Life and Source Term and Total System Performance Assessment and Integration Issue Resolution Status Reports state colloids likely of low influence but recommend continued modeling (Total System Performance Assessment for the Site Recommendation confirms low influence)

Reference: *Total System Performance Assessment for Site Recommendation,* TDR-WIS-PA-000001, Figure 3.5-20

C05

Summary

- **In-package chemistry component new in Total System Performance Assessment for the Site Recommendation**
  - Added to isolate uncertainty caused by in-package chemistry and further understanding
  - Further improvements in most current revision of Analysis Model Report (ANL-EBS-MD-000001 Rev 01) to improve the technical basis
- **Colloid concentration component greatly improved in Total System Performance Assessment for the Site Recommendation**
  - Colloids have remained minor contributor to the overall dose

Colloid Concentration

- **NRC comment**
  - Provide stronger technical basis for exclusion of colloids from spent nuclear fuel
- **Basis for Resolution**
  - Testing is underway to examine existing drip tests to enhance technical basis; findings will be reported in future revision of *Waste Form Colloid-Associated Concentration Limits: Abstraction and Summary Analysis/Model Report,* ANL-WIS-MD-000012

Exclusion of Geochemical, Radiolytic, and Coupled THC Effects

- **NRC Comment**
  - Provide stronger technical basis for exclusion of geochemical, radiolytic, and coupled thermal-hydrological-chemical effects other than pH and ionic strength
- **Basis for Resolution**
  - pH and ionic strength are dominant processes
  - Two other potentially important factors were conservatively omitted: (a) presence of different mineral colloids with different surface charges, and (b) simultaneous consideration of different types of colloids
  - Other processes such as elevated temperatures and convection cells may stabilize colloids for a while but do not exist a short distance from the waste package

References: *Waste Form Degradation PMR*, TDR-WIS-MD-000001, and *Waste Form Colloid-Associated Concentration Limits: Abstraction and Summary AMR*, ANL-WIS-MD-000012

Exclusion of Geochemical, Radiolytic, and Coupled THC Effects (Continued)

- **Basis for Resolution (Continued)**
  - The primary effect of radiolysis is to lower the pH in localized environments. For colloid stability, bulk chemistry, as calculated by the In-Package Component, is appropriate to use since the colloids must travel through many microenvironments; the average of these microenvironments is best represented by the bulk chemistry. Production of small acidic environments by radiolysis does not dominant the bulk chemistry defined by waste form and waste package content degradation
  - Radiolysis effects on waste form and cladding degradation addressed as features, events, and processes and discussed during the Technical Exchange on Container Life and Source Term
  - Future revision to *Waste Form Colloid-Associated Concentration Limits: Abstraction and Summary Analysis/Model Report* (ANL-WIS-MD-00012) will more explicitly state these arguments when excluding geochemical, radiolytic, and coupled thermal-hydrological-chemical processes

Colloidal Formation and Transport

- **NRC Comment**
  - State which radionuclides are included, provide a technical basis, and provide relevant model parameters
- **Basis for Resolution**
  - Even with conservative assumptions, colloids are not major contributors to the dose
  - Pu and Am are the primary radionuclides
  - Pa and Th also included because they are important daughters
  - Qualitative reasoning for selecting radionuclides provided in *Waste Form Colloid-Associated Concentration Limits: Abstraction and Summary Analysis/Model Report* (ANL-WIS-MD-00012)

Colloidal Formation and Transport
(Continued)

- **NRC Comment**
  - Provide reasonable assurance that the adopted maximum concentration of irreversibly attached Pu is bounding
- **Basis for Resolution**
  - Maximum concentration re-evaluated recently (only a slight adjustment was made on maximum)
  - Lower range now provided
  - DOE will provide updated information in future revision to *Waste Form Colloid-Associated Concentration Limits: Abstraction and Summary Analysis Model Report* (ANL-WIS-MD-00012)

Colloidal Formation and Transport
(Continued)

- **NRC Comment**
  - Evaluate the effect of alternative colloid release model described in the analysis model report
- **Basis for Resolution**
  - Although an alternative model was described, data necessary to develop parameters was not available
  - A more conservative model for which parameters could be developed was selected

Conclusions

- DOE considers that NRC comments about colloidal formation and transport related to Subissue 3 have been addressed. The information presented and the planned studies to confirm expectations about colloid-associated concentration limits support a status of Closed-Pending for Subissue 3

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

Total System Performance Assessment Representation of Effects of Coupled Thermal-Hydrological-Chemical Processes on Radionuclide Transport for Subissue 4

Presented to:
DOE/NRC Technical Exchange on Key Technical Issue and Subissues Related to Evolution of the Near-Field Environment

Presented by:
Mike Gross
Civilian Radioactive Waste Management System Management and Operating Contractor

January 9-12, 2001
Pleasanton, CA

YUCCA MOUNTAIN PROJECT

Outline

- Presentation Objectives
- Current Subissue Status
- No NRC comments have been identified for Evolution of the Near-Field Environment Subissue 4 related to radionuclide transport in the Engineered Barrier System
- Conclusions

Presentation Objectives

- **This presentation will summarize the Total System Performance Assessment representation of coupled thermal-hydrological-chemical processes in the Engineered Barrier System. This representation combines**
  - Abstractions for coupled thermal-hydrological-chemical processes in the drift
  - Transport algorithms in the Engineered Barrier System

Total System Performance Assessment Approach to Thermal-Hydrological-Chemical Effects on Transport

- **The Engineered Barrier System transport abstraction combines abstractions for coupled thermal-hydrological-chemical response of engineered barrier system components and environments**
  - In-drift thermal-hydrological and seepage abstractions provide the thermal and hydrological environments in which transport takes place
    - Seepage rate
    - Drip shield temperature
    - Saturation of the invert
    - Evaporative flux from the invert

Total System Performance Assessment Approach to Thermal-Hydrological-Chemical Effects on Transport (Continued)

- **The Engineered Barrier System transport abstraction combines abstractions for coupled thermal-hydrological-chemical response of Engineered Barrier System components and environments**
  - Corrosion of the waste package and drip shield creates fluid flow paths to and from the source of radionuclides
    - Time-dependent growth of stress corrosion cracks and patches
  - Radionuclide source term for dissolved species and colloids
    - Dissolution rates
    - Solubility limits
    - Colloidal concentrations

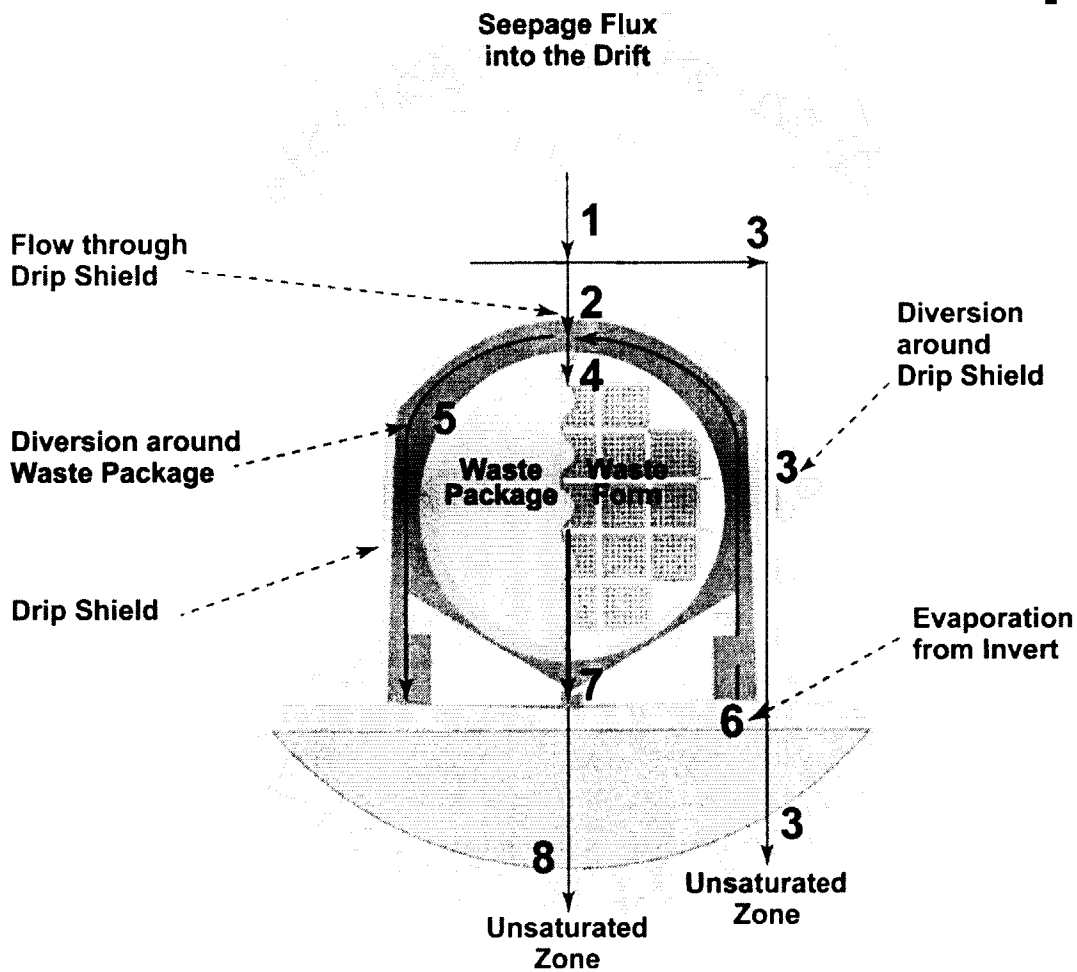
Engineered Barrier System Transport Abstraction Model Assumptions

- **Diffusive transport begins when stress corrosion cracks form in the waste package**
  - Waste form and stress corrosion cracks always wetted with a thin film
  - Thermal effects (dryout) not included
- **Mobilized radionuclides are immediately available to diffuse through stress corrosion cracks (and patches)**
  - Waste package in contact with the invert
- **Invert diffusion coefficient is**
  - Bounded by self-diffusion of water
  - Corrected for porosity, saturation, and temperature

Engineered Barrier System Transport Abstraction Model Assumptions (Continued)

- **Advective flow occurs through patches formed by general corrosion**
- **Advective flow does not occur through stress corrosion cracks**
  - Surface tension will prevent droplets from passing through cracks
- **No retardation in the Engineered Barrier System**
  - Corrosion products are a potential sorber for many radionuclides
- **Longitudinal and transverse dispersion ignored**
  - Effects negligible within the Engineered Barrier System

Total System Performance Assessment Approach to Thermal-Hydrological-Chemical Effects on Transport



abq0063G385.ai

Reference: *EBS Radionuclide Transport Abstraction* (ANL-WIS-PA-000001)

Engineered Barrier System Transport Abstraction Model Assumptions (Continued)

- **Flow-through model for the waste package**
  - Conservative for release of radionuclides relative to a "bathtub" model
- **One-dimensional, quasi-static flow**
  - Consistent with flow-through model
- **Drip shield remains intact**
  - Thermal expansion, rockfall, floor heave, and seismic events will not compromise drip shield as a flow barrier

Radionuclide Solubility and Colloid Stability Set Upper Limits on Radionuclide Concentrations Leaving the Invert

- **Chemical environment for application of solubility and colloid stability limits**
  - Taken from abstractions of calculated water compositions applicable on drip shield, on waste package, and in invert
    - Pitzer approach for stepwise evaporation and equilibration - technical basis for equilibrium assumption to be presented
    - Using inputs of local in-drift evaporation rates, relative humidities, and temperatures from thermal-hydrological abstractions
    - Using inputs of seepage rates, seepage compositions, and CO_2 in gas from seepage and thermal-hydrological-chemical abstractions

References

- **In-Drift Thermal-Hydrological Conditions**
  - Multi-Scale Thermohydrologic Model (ANL-EBS-MD-000049)
  - Abstraction of NFE Drift Thermodynamic Environment and Percolation Flux (ANL-EBS-HS-000003)
- **In-Drift Seepage**
  - Seepage Model for PA Including Drift Collapse (MDL-NBS-HS-000002)
  - Abstraction of Drift Seepage (ANL-NBS-MD-000005)
- **Waste Package Degradation**
  - WAPDEG Analysis of Waste Package and Drip Shield Degradation (ANL-EBS-PA-000003)
- **Colloids**
  - In-Drift Colloids and Concentrations (ANL-EBS-MD-000042)
  - Waste Form Colloid-Associated Concentrations Limits: Abstraction and Summary (ANL-WIS-MD-000012)
- **Flow And Transport**
  - Invert Diffusion Properties Model (ANL-EBS-MD-000031)
  - EBS Radionuclide Transport Abstraction (ANL-WIS-PA-000001)

Conclusions

- **The Engineered Barrier System Radionuclide Transport Abstraction provides a valid basis for Total System Performance Assessment for the Site Recommendation**
  - Conservative representation for transport of dissolved species and colloids
  - Abstractions of process-level models provide the appropriate thermal-hydrological-chemical responses of in-drift components
- **DOE considers that NRC comments discussed in this presentation have been addressed and that this information supports a status of Closed-Pending for Subissue 4**

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

NRC Comments on Coupled Thermal-Hydrological-Chemical Processes Affecting the Calico Hills Hydrogeological Unit Related to Subissue 1

Presented to:
DOE-NRC Technical Exchange on Key Technical Issue and Subissues Related to Evolution of the Near-Field Environment

Presented by:
Eric Sonnenthal
John A. Apps
Civilian Radioactive Waste Management System Management and Operating Contractor

January 9-12, 2001
Pleasanton, CA

YUCCA MOUNTAIN PROJECT

Outline

- **Presentation Objectives**
- **Current Subissue Status**
- **For NRC comments on coupled processes related to Subissue 1, Evolution of the Near-Field Environment, Key Technical Issue, this presentation will**
  - Summarize technical basis for item resolution
  - Identify basis documents (References)
  - Summarize technical adequacy of basis
- **References**
- **Conclusions**

Presentation Objectives

- **Describe the basis for resolving NRC comments on thermal-hydrological-chemical processes affecting the Calico Hills nonwelded hydrogeological (CHn) unit related to Subissue 1 of the Evolution of the Near Field Environment Key Technical Issue**
- **DOE has tentatively determined**
  - Changes in the CHn unit caused by coupled thermal-hydrological-chemical processes will be inconsequential because the duration and magnitude of the thermal pulse and kinetic factors affecting the metastabilities of extant phases are too small to cause significant alteration (Drift-Scale Coupled Processes (DST and THC Seepage) Models Analysis/Model Report, MDL-NBS-HS-000001 Rev 01, in review)
  - Coupled thermal-hydrological-chemical effects on the CHn can be excluded from Total System Performance Assessment for the Site Recommendation because the effects are negligible

Current Subissue Status

- **Evolution of the Near-Field Environment Issue Resolution Status Report, Rev 03, indicates that Subissue 1 is OPEN**

Effects of THC Processes on the CHn

- **NRC Comments**
  - Evaluate the effects of loss of water from the alteration of clinoptilolite to analcime
  - Provide technical basis for excluding coupled thermal-hydrological-chemical effects on the CHn from Total System Performance Assessment for the Site Recommendation
    - Thermal-hydrological-chemical processes that could adversely affect the natural barrier properties due to a transient thermal excursion to ~70° C include
    - Mineral alteration with adverse changes in the sorptive properties of zeolites with respect to radionuclides
    - Consequent changes in porosity and permeability
    - Release of zeolitic waters of hydration with or without zeolitic phase changes

Effects of THC Processes on the CHn
(Continued)

- **Basis for Resolution**
  - The following preliminary findings are based on thermal-hydrological-chemical modeling and earlier literature studies
    - Maximum thermal excursion is to about 70°C (Drift-Scale Coupled Processes (DST and THC Seepage) Models Analysis/Model Report, MDL-NBS-HS-000001 Rev 01, in review)
    - Resulting porosity, permeability, and mineralogical changes in the CHn are expected to be inconsequential (Drift-Scale Coupled Processes (DST and THC Seepage) Models Analysis/Model Report, MDL-NBS-HS-000001 Rev 01, in review)

Effects of THC Processes on the CHn
(Continued)

- **Basis for Resolution (Continued)**
  - Alteration of clinoptilolite to analcime is not expected
    - Non-equilibrium water/rock interactions - I. Model for Interface–Controlled Reactions
    - Kinetic Model of Zeolite Paragenesis in Tuffaceous Sediments
    - Kinetics of Silica-Phase Transitions
    - Preliminary Conceptual Model for Mineral Evolution in Yucca Mountain
  - Mountain-scale thermal-hydrological-chemical modeling now under consideration, is expected to verify the preliminary results

Effects of Loss of Water from Alteration of Clinoptilolite to Analcime

- **Basis for Resolution**
  - The alteration of clinoptilolite to analcime is believed to be a kinetically controlled process described by the Ostwald Rule of Stages
  - The reaction can be written as:
    $s\text{Clinoptilolite} + t\text{Na}^+ \Leftrightarrow v\text{Analcime} + w\text{K}^+ = x\text{Ca}^{2+} = y\text{SiO}_2 + z\text{H}_2\text{O}$

Effects of Loss of Water from Alteration of Clinoptilolite to Analcime (Continued)

- **Basis for Resolution (Continued)**
  - Factors affecting the rate of transformation include:
    - The solid state diffusive rate of ordering of opal-CT
    - Nucleation and growth of secondary quartz
    - Advective removal of dissolved silica
    - Extent of substitution of Na^+ and K^+ by Mg^{2+} and Ca^{2+} in clinoptilolite
    - Stoichiometry of analcime
    - Composition and salinity of the aqueous phase
    - Temperature

Effects of Loss of Water from Alteration of Clinoptilolite to Analcime (Continued)

- **Basis for Resolution (Continued)**
  - Information from relevant published literature indicates
    - Changes in percolation flux in the CHn after emplacement of waste are expected to be insufficient to materially affect advective removal of dissolved silica, even taking into account the increased solubility of opal-CT, zeolites, and clays (Drift-Scale Coupled Processes (DST and THC Seepage) Models Analysis/Model Report, MDL-NBS-HS-000001 Rev 01, in review)
    - The duration and magnitude of the thermal excursion in the CHn are expected to be insufficient to cause alteration of more than 10 percent opal-CT to quartz (Preliminary Conceptual Model for Mineral Evolution in Yucca Mountain LA-12708-MS)

Effects of Loss of Water from Alteration of Clinoptilolite to Analcime (Continued)

- **Basis for Resolution (Continued)**
  - Information from relevant published literature indicates
    - Silica dissolution in the repository horizon is expected to saturate some of the water percolating into the CHn with respect to amorphous silica. This water would inhibit recrystallization of opal-CT to quartz (Drift-Scale Coupled Processes (DST and THC Seepage) Models Analysis/Model Report, MDL-NBS-HS-000001 Rev 01, in review)
    - Maintenance of an elevated silica activity would stabilize clinoptilolite and inhibit analcime formation (Preliminary Conceptual Model for Mineral Evolution in Yucca Mountain LA-12708-MS and Equilibrium Modeling of Clinoptilolite-Analcime Equilibria at Yucca Mountain, Nevada (Clays and Clay Minerals, 45, (2), 226-239)

Effects of Loss of Water from Alteration of Clinoptilolite to Analcime (Continued)

- **Basis for Resolution (Continued)**
  - Quantification of the effects of water loss from alteration of clinoptilolite to analcime is expected during mountain-scale thermal-hydrological-chemical process simulations now being considered
- **References**
  - Drift-Scale Coupled Processes (DST and Seepage) Models Analysis Model Report, MDL-NBS-HS-000001 Rev 01, in review
  - Distribution and Chemistry of Diagenetic Minerals at Yucca Mountain, Nye County, Nevada
  - Equilibrium Modeling of Clinoptilolite-Analcime Equilibria at Yucca Mountain, Nevada
  - Kinetic Model of Zeolite Paragenesis in Tuffaceous Sediments

Effects of Loss of Water from Alteration of Clinoptilolite to Analcime (Continued)

- **References (Continued)**
  - Kinetics of Silica Phase Transitions
  - Preliminary Conceptual Model for Mineral Evolution in Yucca Mountain

Exclusion of Coupled THC Effects on the CHn from Total System Performance Assessment for the Site Recommendation

- **Basis for Resolution (Continued)**
  - Preliminary findings, based on information from thermal-hydrological-chemical seepage modeling and relevant published literature include
    - THC Seepage Modeling (Drift-Scale Coupled Processes (DST and Seepage) Models Analysis/Model Report, MDL-NBS-HS-000001 Rev 01, in review) and information from preliminary studies indicates that no more than 0.5 percent of the extant zeolites would alter to other zeolites stable in a high silica activity environment
    - Total porosity changes would be less than one percent (MDL-NBS-HS-000001 Rev 01)
    - Permeability changes would be negligible (MDL-NBS-HS-000001 Rev 01)

Exclusion of Coupled THC Effects on the CHn from Total System Performance Assessment for the Site Recommendation (Continued)

- **Basis for Resolution (Continued)**
  - Effects of temperature on the ion exchange properties of clinoptilolite and mordenite are expected to be relatively minor
  - Minor changes in the water of hydration of the principal zeolites would occur, but would not be expected to significantly affect radionuclide sorption behavior because changes in the radionuclide concentrations in the aqueous phase would be small
    - » Calorimetric Measurement of the Enthalpy of Hydration of Clinoptilolite
    - » Equilibrium in the Clinoptilolite-H_2O System

Exclusion of Coupled THC Effects on the CHn from Total System Performance Assessment for the Site Recommendation (Continued)

- **Basis for Resolution (Continued)**
  - Alteration of clinoptilolite to analcime would not be expected
    - Drift-Scale Coupled Processes (DST and THC Seepage) Models Analysis/Model Report, MDL-NBS-HS-000001 Rev 01, in review
    - Kinetic Model of Zeolite Paragenesis in Tuffaceous Sediments
    - Preliminary Conceptual Model for Mineral Evolution in Yucca Mountain
    - Equilibrium in the Clinoptilolite-H_2O System
  - Quantification is expected from the mountain-scale thermal-hydrological-chemical process simulations

Exclusion of Coupled THC Effects on the CHn from Total System Performance Assessment for the Site Recommendation (Continued)

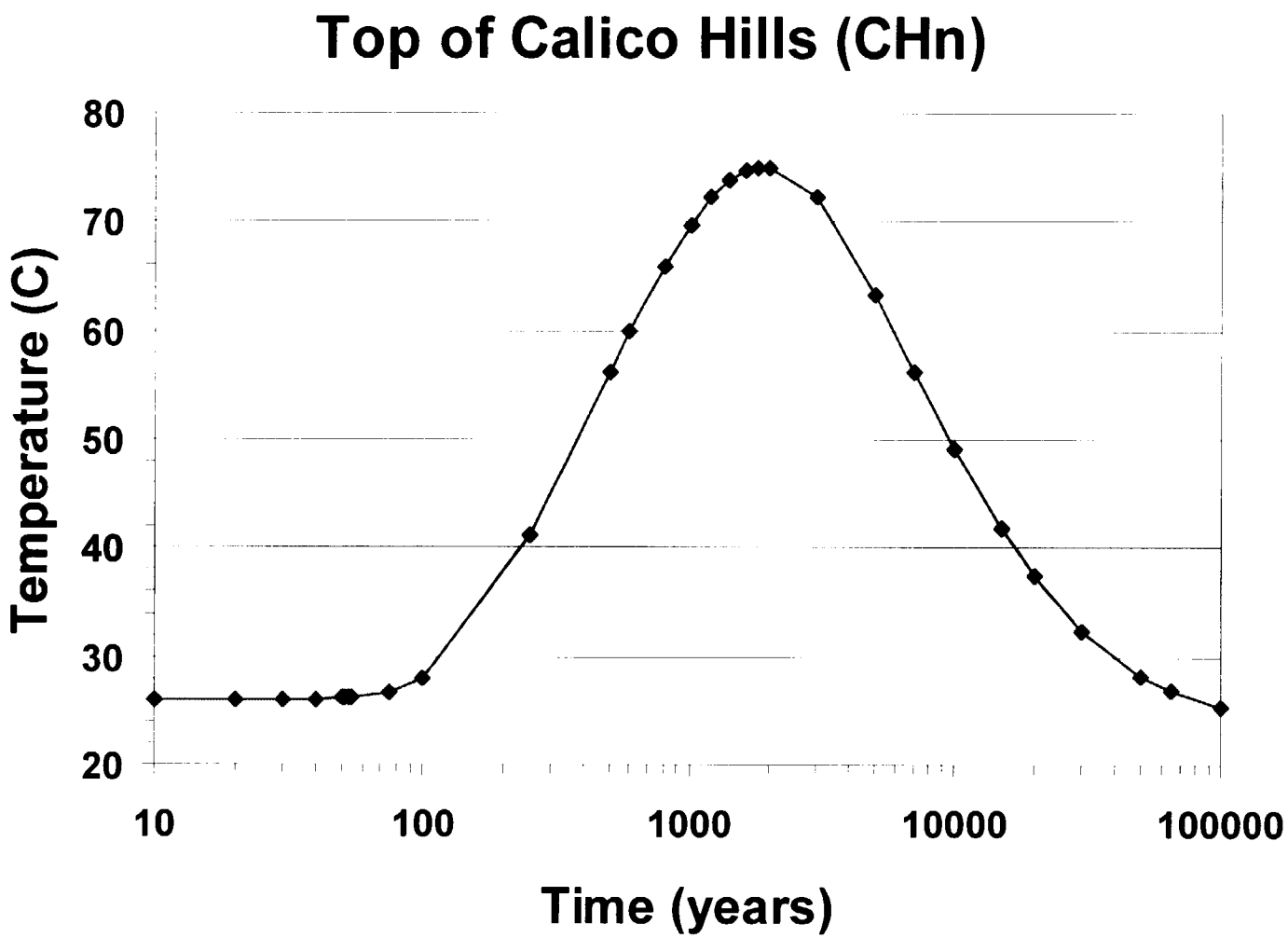
- **References**
  - Drift-Scale Coupled Processes (DST and THC Seepage) Models Analysis/Model Report, MDL-NBS-HS-000001 Rev 01, in review
  - Non-Equilibrium Water/Rock Interactions - I. Model for Interface-Controlled Reactions
  - Kinetic Model of Zeolite Paragenesis in Tuffaceous Sediments Preliminary Conceptual Model for Mineral Evolution in Yucca Mountain
  - Calorimetric Measurement of the Enthalpy of Hydration of Clinoptilolite
  - Equilibrium in the Clinoptilolite-H_2O System

Conclusions

- **Effects of loss of water from the alteration of clinoptilolite to analcime are expected to be minor because extensive alteration of clinoptilolite to analcime is not expected**
- **Thermal-hydrological-chemical effects on the CHn can be excluded from Total System Performance Assessment**
  - Preliminary evaluations indicate that only small amounts of zeolites will alter to other zeolites that are stable in a high silica environment
  - Total porosity and permeability changes will be minor
- **DOE considers NRC comments about alteration of the CHn and related to Subissue 1 have been addressed. This presentation and the additional studies being considered to confirm expectations about mountain-scale thermal-hydrological-chemical effects support a status of Closed-Pending for Subissue 1**

Backup Slides

Temperatures at the Top of the CHn



Temperature as a function of time at the top of the CHn hydrologic unit

Reference: Drift-Scale Coupled Processes (DST and THC Seepage) Models Analysis Model Report MDL-NBS-HS-000001 Rev 01, in review

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

Subissue 1: NRC Comments on Thermal Alteration of the Paintbrush Tuff Nonwelded Hydrogeologic Unit

Presented to:
DOE-NRC Technical Exchange on Key Technical Issue and Subissues Related to Evolution of the Near-Field Environment

Presented by:
Nicolas Spycher
Civilian Radioactive Waste Management System Management and Operating Contractor

January 9-12, 2001
Pleasanton, CA

YUCCA MOUNTAIN PROJECT

Outline

- **Presentation Objectives**
- **Current Subissue Status**
- **For NRC Comments on thermal alteration of the Paintbrush Tuff nonwelded hydrogeologic unit related to Subissue 1 of the Evolution of the Near-Field Environment Key Technical Issue, this presentation will**
  - Summarize technical basis for item resolution
  - Identify basis documents (References)
  - Summarize technical adequacy of basis
- **Conclusions**

Presentation Objectives

- Provide basis for resolving NRC comments on thermal alteration of the Paintbrush Tuff nonwelded hydrogeologic unit associated with Subissue 1
- DOE has considered the technical basis for neglecting the thermal alterations to the Paintbrush Tuff nonwelded hydrogeologic unit
- DOE has determined that the effects of alteration of the Paintbrush Tuff nonwelded hydrogeologic unit on performance assessment would be negligible

Current Subissue Status

- Evolution of The Near Field Environment Issue Resolution Status Report, Rev 03 indicates Subissue 1 status is OPEN

Total System Performance Assessment Treatment of Subissue 1

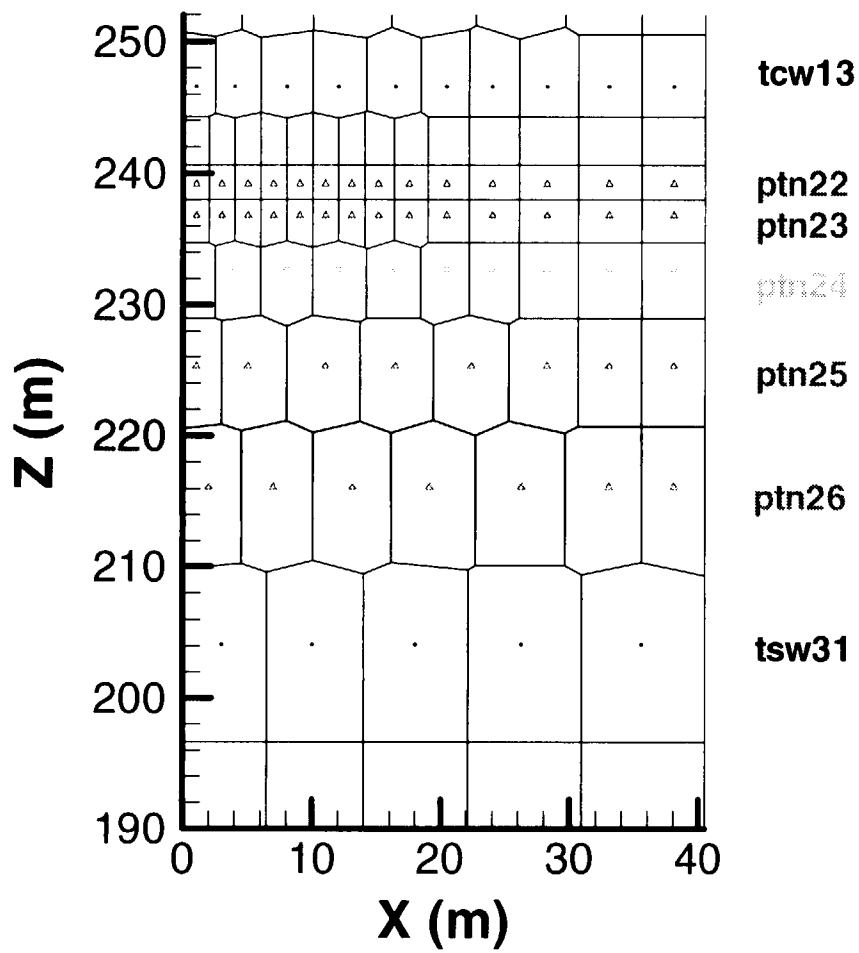
- **NRC Comments**
  - Provide the technical basis for neglecting alteration of the Paintbrush Tuff nonwelded hydrogeologic unit unit
  - Evaluate the importance of alteration to performance
- **Basis for Resolution**
  - Porosity in the Paintbrush Tuff nonwelded hydrogeologic unit is large, so mineral precipitation and dissolution have little effect on flow in this unit and are unimportant to Total System Performance Assessment modeling (Drift-Scale Coupled Processes (DST and THC Seepage) Models Analysis/Model Report, MDL-NBS-HS-000001 Rev 02, work in progress)
  - Thermal-Hydrological-Chemical Seepage Model predicts negligible porosity and permeability changes due to chemical alteration of the Paintbrush Tuff nonwelded hydrogeologic unit (MDL-NBS-HS-000001 Rev 02, work in progress)
  - Supporting model data will be submitted with the Drift-Scale Coupled Processes Analysis/Model Report Rev 01, in review. Specifically addressed in Rev 02

Process Modeling

- **Basis for Resolution**
  - Thermal-hydrological-chemical seepage models incorporate the Paintbrush Tuff nonwelded hydrogeologic unit
  - Thermal-hydrological-chemical effects, including mineral alteration and porosity change in both fractures and matrix of the Paintbrush Tuff nonwelded hydrogeologic unit, have been predicted
  - Thermal-hydrological-chemical seepage model results show no significant alteration effects on flow in the Paintbrush Tuff nonwelded hydrogeologic unit
  - Simulations yield consistent ambient water compositions within the range of field observations, providing an indication that modeled mineral and glass reaction rates and compositions are reliable
  - Sensitivity analyses on glass reaction rate, composition, and thermodynamic properties will be performed as part of planned mountain-scale simulations to reduce prediction uncertainty, and are expected to confirm results of the thermal-hydrological-chemical seepage models

Process Modeling
(Continued)

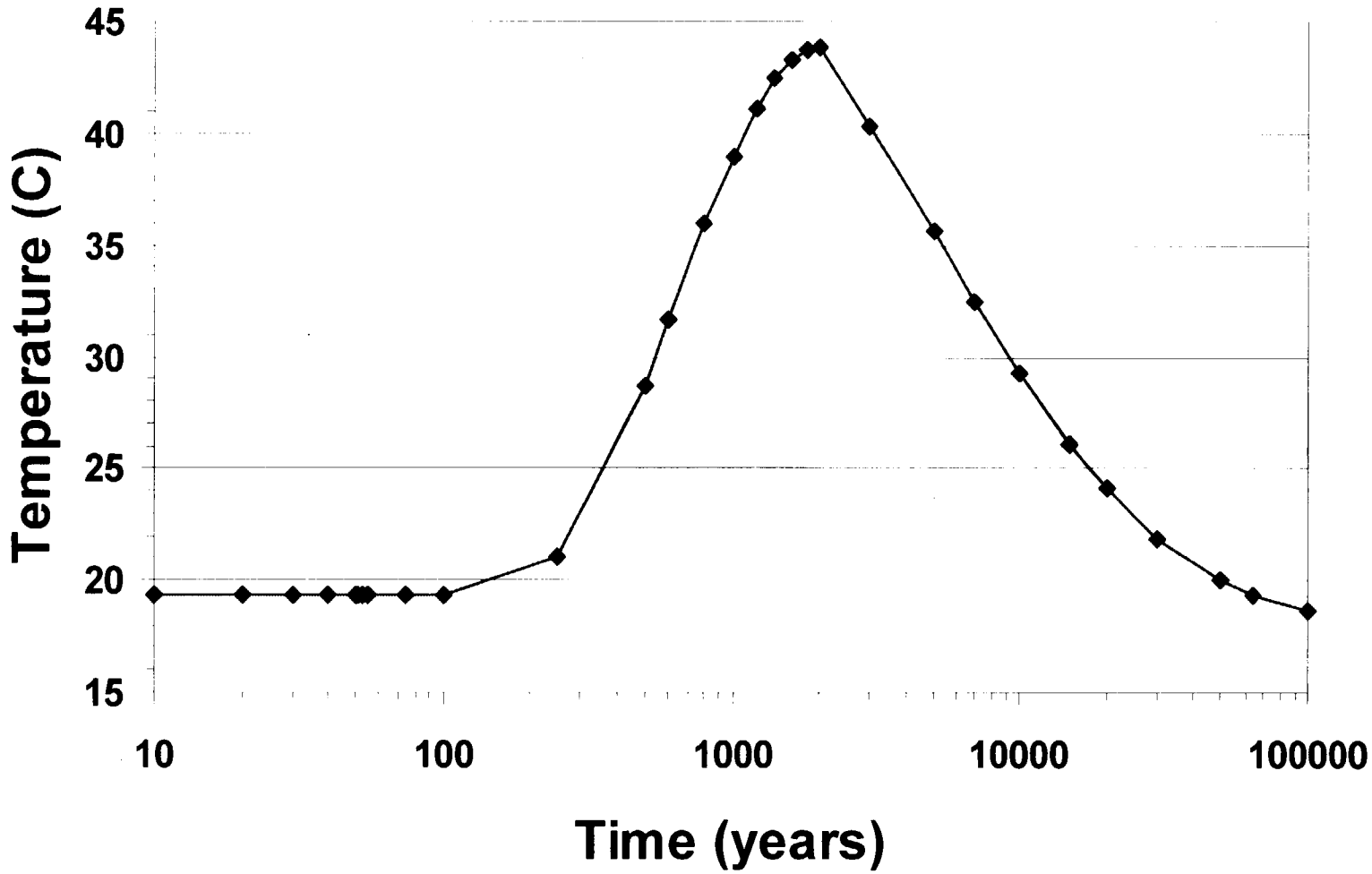
THC Seepage Model
PTn Hydrogeologic Unit



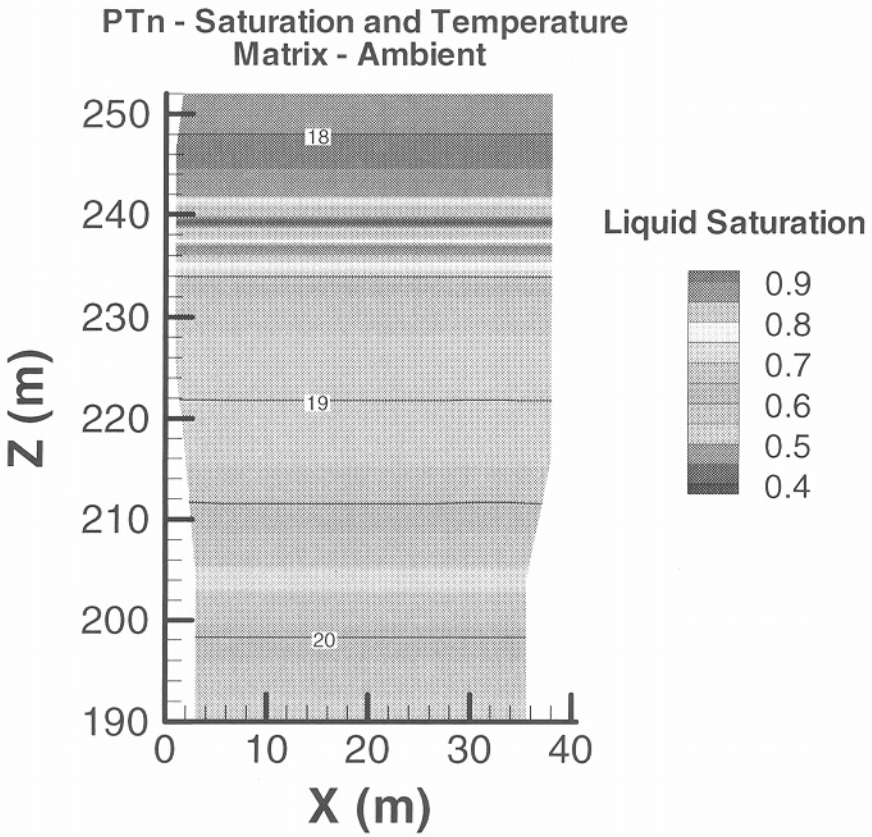
Reference: Drift-Scale Coupled Processes AMR - MDL-NBS-HS-000001 Rev 02, work in progress

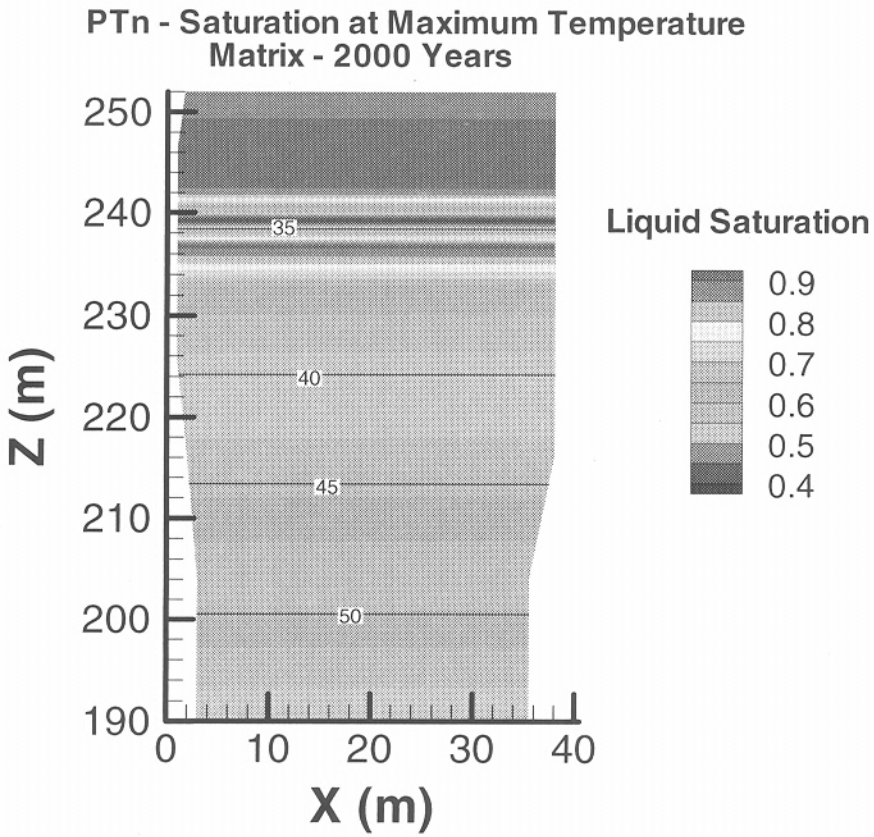
Process Modeling
(Continued)

Bottom of PTn Unit



Process Modeling
(Continued)

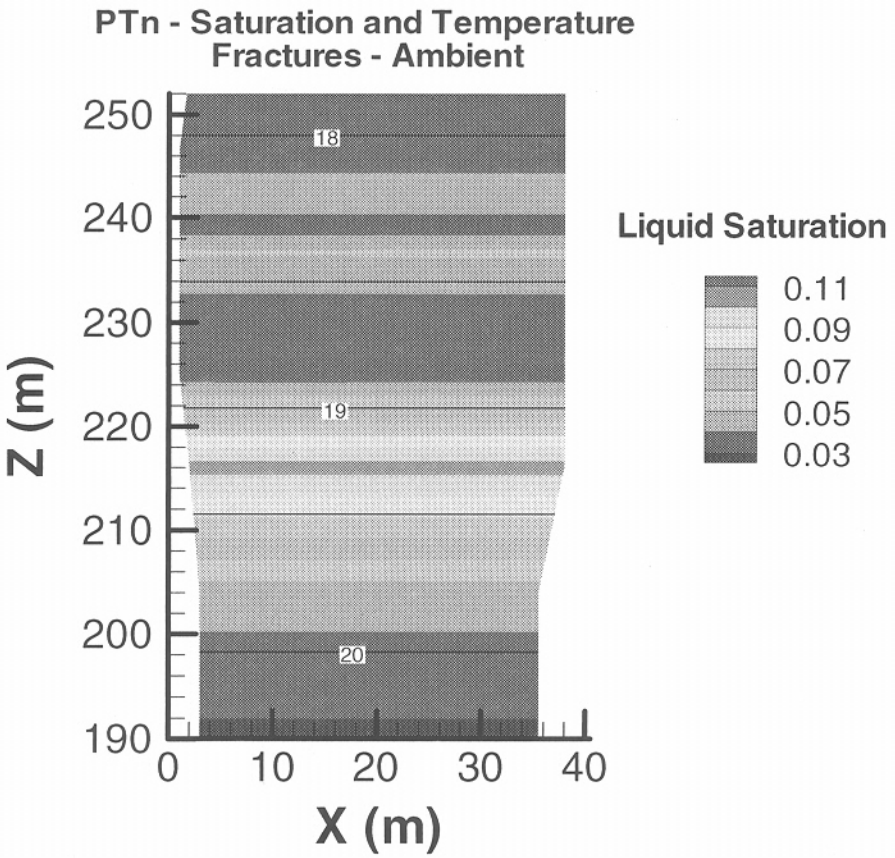


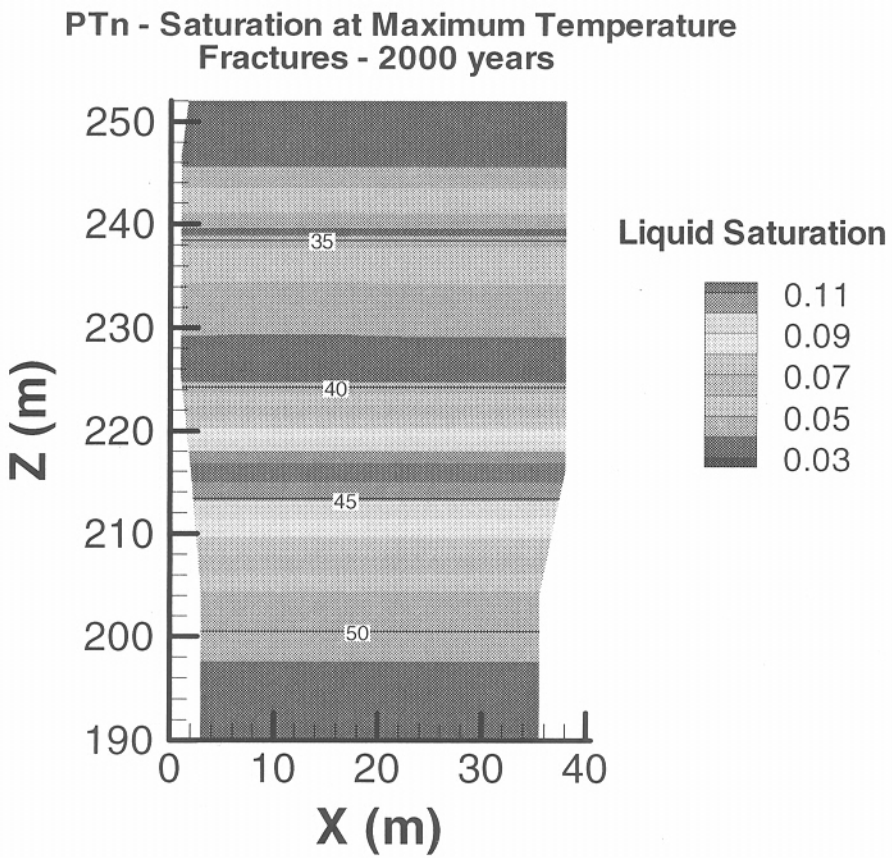


Reference: Drift-Scale Coupled Processes AMR - MDL-NBS-HS-000001 Rev 02 , work in progress

C06

Process Modeling
(Continued)

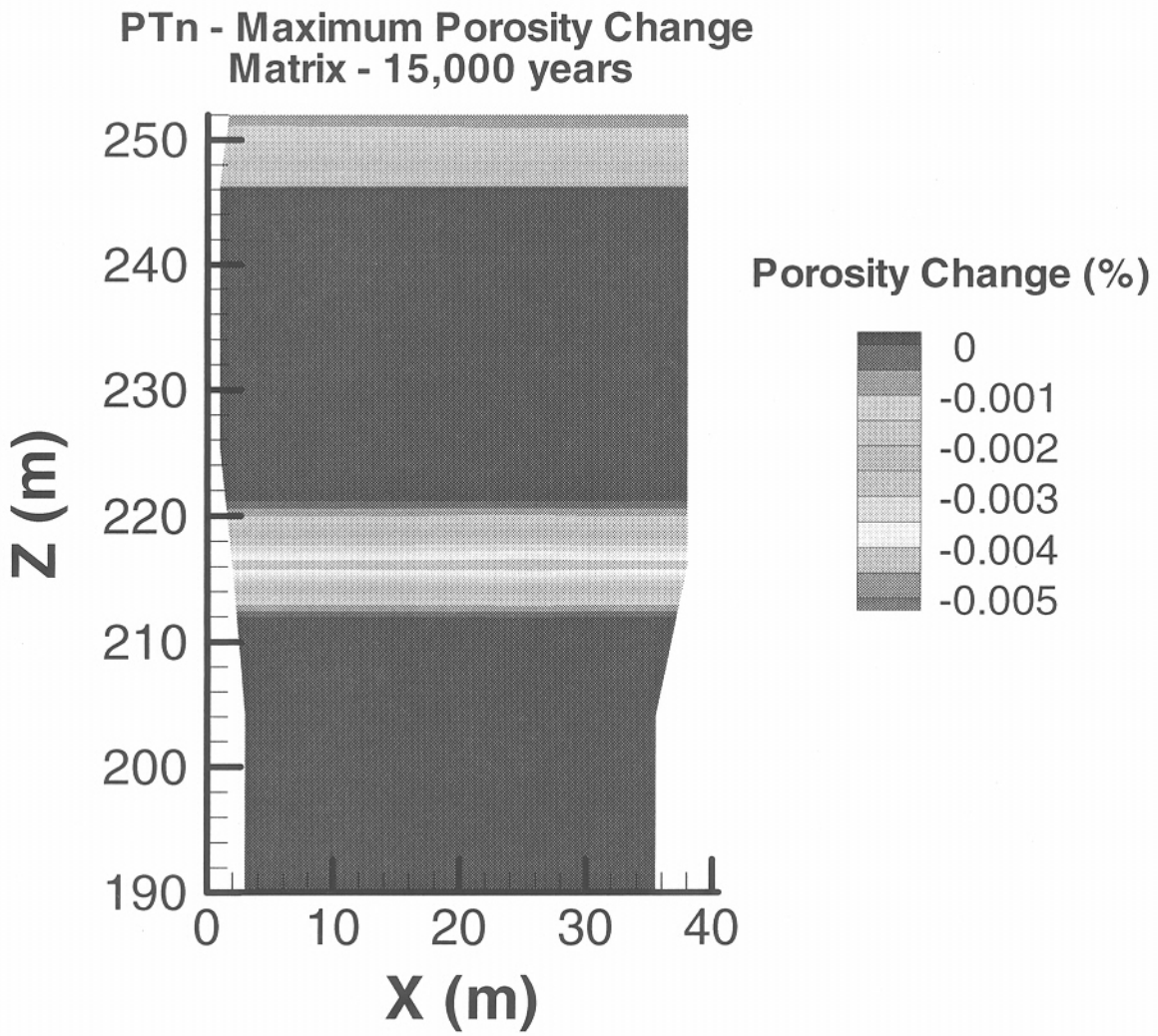




Reference: Drift-Scale Coupled Processes AMR - MDL-NBS-HS-000001 Rev 02 , work in progress

C07

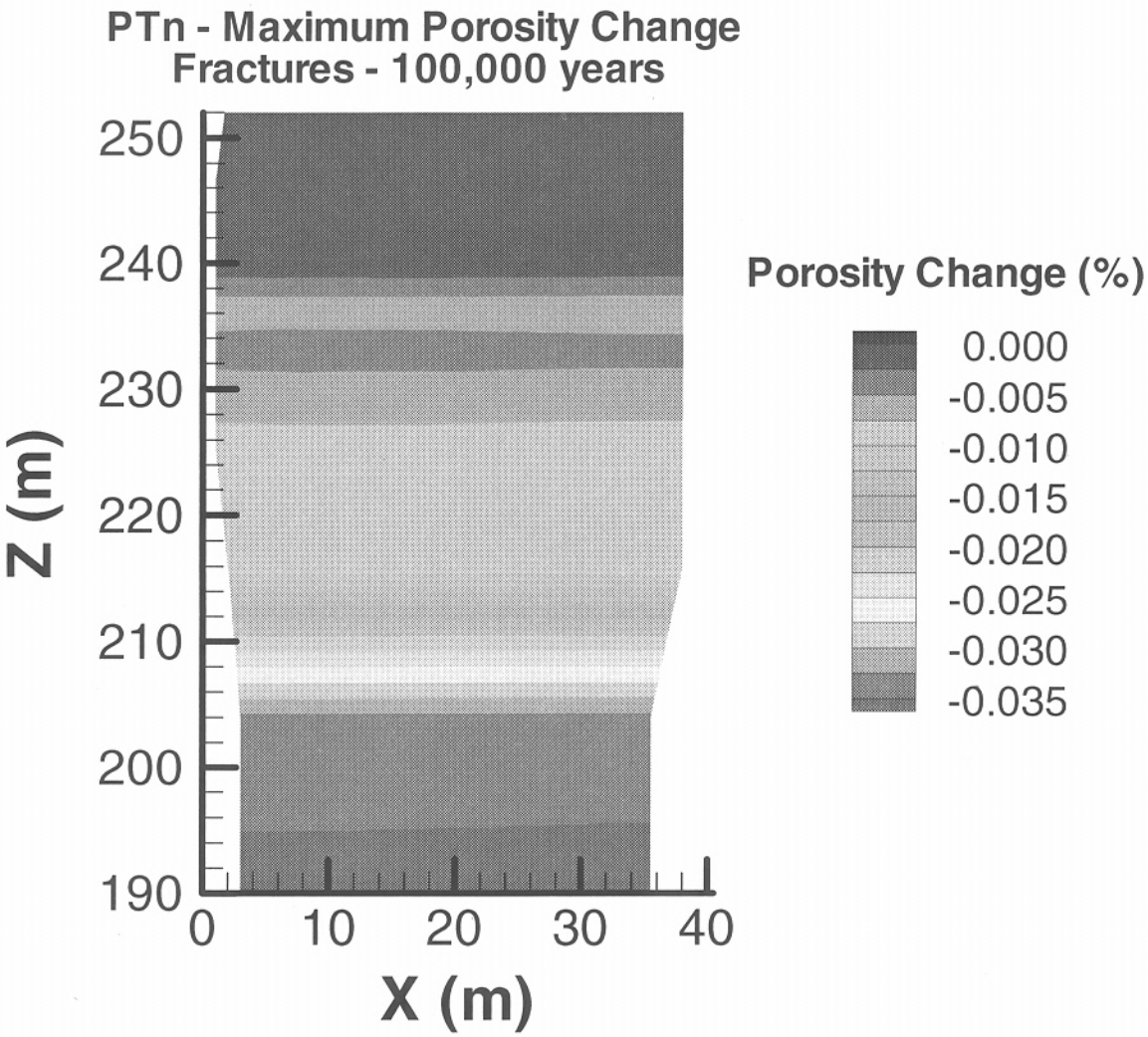
Process Modeling
(Continued)



Reference: Drift-Scale Coupled Processes AMR - MDL-NBS-HS-000001 Rev 02 , work in progress

C08

Process Modeling
(Continued)



Reference: Drift-Scale Coupled Processes AMR-MDL-NBS-HS-000001 Rev 02 , work in progress

C09

Summary

- **Maximum temperature at base near 45°C at 2000 years (Heat Load in Tptpll, No-Backfill 2-D Column Model)**
- **Calculated porosity change is negative (mineral precipitation)**
  - Matrix: maximum < 0.005 % at 15,000 years (calcite and clays)
    Fractures: maximum < 0.02 % at 100,000 years (calcite)
- **Glass dissolution very small**
- **Negligible effect of dissolution/precipitation on flow**
- **Glass chemical and thermodynamic properties are uncertain. However, these data can be constrained with simulations of ambient conditions**

Summary
(Continued)

- Sensitivity analyses are being considered as part of the development of Mountain-Scale Model and are expected to confirm the negligible effect of dissolution and precipitation on flow

References

- Drift-Scale Coupled Processes (Drift-Scale Coupled Processes (DST and THC Seepage) Models Analysis/Model Report, MDL-NBS-HS-000001 Rev 01, is in review)
  - (Simulation results, including predicted thermal-hydrological-chemical parameters in the Paintbrush Tuff nonwelded hydrogeologic unit, were submitted with Rev 01. This item will be addressed in Rev 02)
- Abstraction of Drift Scale Coupled Processes Analysis Model Report (ANL-NBS-HS-000029 Rev 00)
- Near-Field Environment Process Model Report (TDR-NBS-MD-000001 Rev 00/ICN 03)
- Unsaturated Zone Flow and Transport Model Process Model Report (TDR-NBS-HS-000002 Rev 00)

Conclusions

- Technical basis exists for excluding thermal alterations to the Paintbrush Tuff nonwelded hydrogeologic unit from the Total System Performance Assessment, and will be documented in Rev 02 of the Drift-Scale Coupled Processes (Drift Scale Test and Thermal-hydrological-chemical Seepage) Models Analysis/Model Report
- Sensitivity analyses are expected to confirm technical basis
- DOE considers that the NRC comments on thermal alteration of the Paintbrush Tuff nonwelded hydrogeological unit (PTn) related to Subissue 1 have been addressed. The information presented and the additional studies that are planned and being considered to confirm expectations regarding the effects of alteration of the PTn on system performance support a status of Closed-Pending of Subissue 1

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

Subissue 1: Comments on Effects of Cementitious Materials

Presented to:
DOE-NRC Technical Exchange on Key Technical Issue and Subissues Related to Evolution of the Near-Field Environment

Presented by:
Ernest Hardin
Civilian Radioactive Waste Management System Management and Operating Contractor

January 9-12, 2001
Pleasanton, CA

YUCCA MOUNTAIN PROJECT

Outline

- **Presentation Objectives**
- **Current Subissue Status**
- **For NRC comments on the effects of cementitious materials related to Subissue 1 of the Evolution of the Near Field Environment Key Technical Issue, this presentation will**
  - Give the technical bases for limiting the effects of concrete on flow and transport in the unsaturated zone
  - Identify planned analyses that will evaluate the potential effects of concrete used in non-emplacement areas
- **Conclusions**

Presentation Objectives

- Provide the basis for resolving NRC comments about the potential for cementitious materials to modify unsaturated zone flow and transport related to Subissue 1 of the Evolution of the Near-Field Environment Key Technical Issue
- Existing models consider the production and chemical evolution of cement grout used in rock bolts, and show that interaction with CO_2 in the environment will neutralize the leachate (Engineered Barrier System: Physical and Chemical Environment Model, ANL-EBS-MD-000033 Rev 01)

Presentation Objectives
(Continued)

- The DOE recognizes the potential for modifications of flow and transport, and plans specific analyses to evaluate the extent to which conditions important to radionuclide transport are modified by the presence of cement

Current Subissue Status

- **Evolution of The Near Field Environment Issue Resolution Status Report, Rev 03 indicates the status of Subissue 1 is Open**

Effects of Cementitious Materials

- **NRC Comment**
  - Need to analyze and evaluate the potential interaction between cementitious materials and the host rock, in the non-waste emplacement areas of the repository as well as waste emplacement areas

Effects of Cementitious Materials
(Continued)

- **Sensitivity Analysis Was Previously Performed for the Viability Assessment (VA)**
  - Sensitivity of radionuclide releases to concrete leachate was evaluated for the VA (Vol. 3, Section 5.4.4; Concrete-Lined Emplacement Drifts) and found to increase dose rate at the biosphere by approximately an order of magnitude
  - The VA repository design included: 1) much more concrete in fully-lined emplacement drifts (increasing CO_2 demand from carbonation reactions), and 2) carbon steel as the outer waste package corrosion-allowance layer.
  - The calculated dose response from sensitivity testing of cement-leachate effects, was strongly affected by waste package failure instigated by alkaline attack on the waste package steel layer, leading to localized waste package failure

Effects of Cementitious Materials
(Continued)

- **Basis for Resolution**
  - Effects from the use of cement grout for rockbolts are considered in current models (Engineered Barrier System Physical and Chemical Environment Model ANL-EBS-MD-000033 Rev. 01)
  - The effects from cement-grouted rockbolts on CO_2 fugacity and water composition in the drifts will be minor
  - Calcite will be deposited in the engineered barrier system, e.g., on the rock roof and drip shield

Effects of Cementitious Materials
(Continued)

- **Basis for Resolution (Continued)**

Comparison of Cement Leachate Composition with Seepage and Evaporatively Concentrated Waters (Abstracted Time Period 2)

Component or Property	Units	Seepage (Period 2)	Seepage @ RH 95%	Cement Leachate	Equilibrated Leachate
Temperature (C)		96	96	96	96
$\log_{10} P_{O2}$ (redox)	None	-0.7	-0.7	-0.7	-0.7
$\log_{10} P_{CO2}$	None	-6.5	-6.5	< -6.5	-6.5
pH	None	8.1	9.47	10.3186	9.2137
$SiO_{2(aq)}$	molal	1.5×10^{-3}	2.554×10^{-3}	1.73×10^{-5}	1.73×10^{-5}
Na^+	molal	1.4×10^{-3}	1.5377	2.19×10^{-3}	2.19×10^{-3}
K^+	molal	8.5×10^{-5}	6.320×10^{-2}	8.50×10^{-5}	8.50×10^{-5}
Ca^{2+}	molal	6.4×10^{-4}	3.591×10^{-3}	9.62×10^{-3}	3.54×10^{-3}
Mg^{2+}	molal	3.2×10^{-7}	5.110×10^{-6}	3.54×10^{-8}	3.54×10^{-8}
HCO_3^-	molal	1.9×10^{-4}	3.867×10^{-5}	6.98×10^{-6}	1.01×10^{-5}
SO_4^{2-}	molal	6.6×10^{-4}	0.1323	3.05×10^{-3}	3.05×10^{-3}
Cl^-	molal	1.8×10^{-3}	1.3384	1.80×10^{-3}	1.80×10^{-3}
F^-	molal	2.5×10^{-5}	9.367×10^{-4}	2.50×10^{-5}	2.50×10^{-5}
Fe^{2+}	molal	7.9×10^{-10}	6.561×10^{-141} C	4.58×10^{-14}	9.30×10^{-15}
Al^{3+}	molal	2.7×10^{-7}	2.418×10^{-8}	1.59×10^{-3}	5.20×10^{-4}

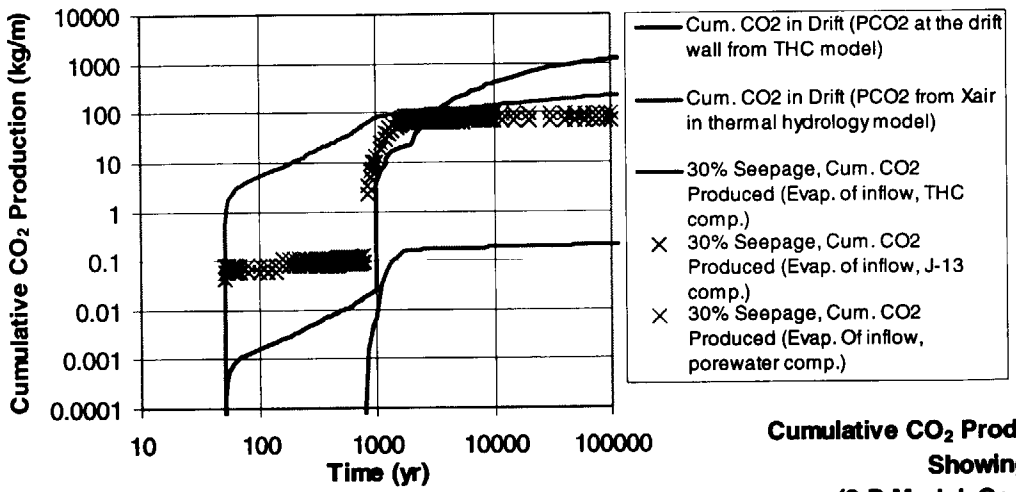
Source: Engineered Barrier System: Physical and Chemical Environment Model ANL-EBS-MD-000033 Rev 01

Effects of Cementitious Materials
(Continued)

- **Basis for Resolution (Continued)**
  - In the existing model for rockbolt cement leachate, a conservative approach to leachate quantity is based on the ratio of the rockbolt cross-sectional area to drift diameter
  - This approach predicts rates of leachate inflow to the drifts, of a few percent of the total seepage (Engineered Barrier System Physical and Chemical Environment Model ANL-EBS-MD-000033 Rev 01)

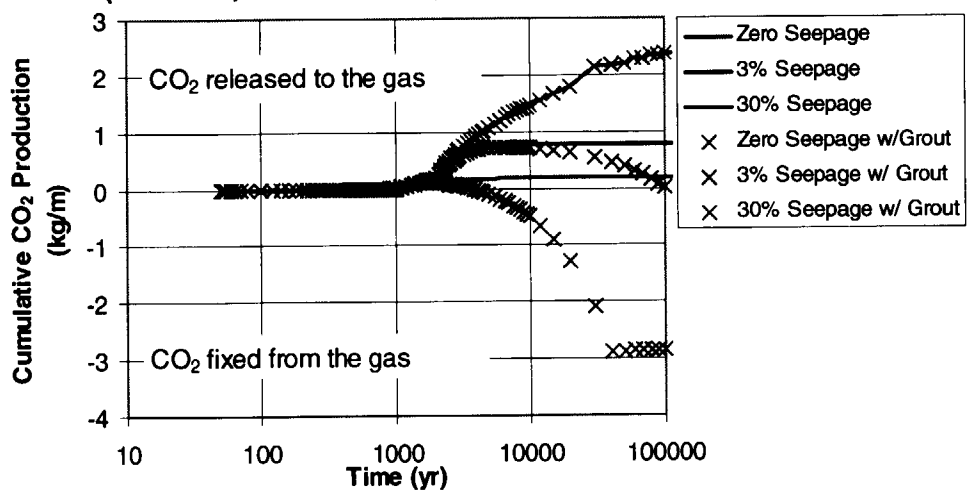
Effects of Cementitious Materials (Continued)

Cumulative CO_2 Production In the Drift from Evaporative Reactions Compared to CO_2 Gas Flow Through Drifts (2-D Model; Center Location; Mean Infiltration)



CO_2 Production in the Emplacement Drift Considering Evaporative Reactions, Compared with Through-Flux from Gas-Phase Circulation

Cumulative CO_2 Production in the Drift from Evaporative Reactions, Showing Effect of Leachate Carbonation (2-D Model; Center Location; Location, Mean Infiltration)



CO_2 Production in the Emplacement Drift from Evaporative Reactions, with Combined Effect from Cement Leachate Carbonation

Source for plots: Engineered Barrier System Physical and Chemical Environment Model ANL-EBS-MD-000033 Rev 01

Effects of Cementitious Materials
(Continued)

- **Basis for Resolution**
  - DOE is considering additional thermal-hydrologic-chemical modeling of interactions between percolating water and concrete-lined shafts, drifts, and stations in the unsaturated zone
    - The thermal-hydrologic-chemical model includes carbon species, and will impose mass balance and gas- and liquid-phase transport constraints to evaluate the nature and extent of neutralization reactions involving CO_2
    - Leaching is represented by dissolution of portlandite and ettringite (Engineered Barrier System Physical & Chemical Environment Analysis Model Report ANL-EBS-MD-000033 Rev 01)

Effects of Cementitious Materials
(Continued)

- **Basis for Resolution (Continued)**
  - Perspectives on Additional Modeling
    - Interactions will be constrained by hydraulic effects such as dispersion, limited permeability, and carbonation reactions
    - Concrete and grout will not generally be present along potential radionuclide transport pathways
      - » Interaction with radionuclides will first require cement- leachate transport and will therefore be indirect
      - » Reaction with gas-phase CO_2 along leachate flow pathways will neutralize pH (based on Engineered Barrier System Physical & Chemical Environment Analysis Model Report, Rev 01)
    - Effects of leachate on host rock properties will be dominated by calcite precipitation that will tend to reduce permeability along flowpaths by which cement leachate can be transport into radionuclide transport pathways
    - The composition and quantity of cement-leachate after equilibration to CO_2 in the unsaturated zone are likely to be of minor importance compared to the composition and quantity of water in the bulk environment

Effects of Cementitious Materials
(Continued)

- **Basis for Resolution (Continued)**
  - Perspectives on Additional Modeling
    - The effects of modified transport path chemistry on radionuclide mobility are expected to be minor
      - » Non-sorbing soluble nuclides (Tc, I) will be unaffected as represented in current models (Unsaturated Zone Flow and Transport Model Process Model Report TDR-NBS-HS-000002 Rev 00 ICN 1, Section 3.11)
      - » Irreversible colloids will be unaffected consistent with current models (Total System Performance Assessment Model TDR-WIS-PA-000001 Rev 00 ICN 01, Section 3.7.1.5)
      - » Concentrations of potential complexing species (e.g. CO_2 species and sulfate) will be moderately elevated (Engineered Barrier System Physical and Chemical Environment Model ANL-EBS-MD-000033 Rev 01)

Effects of Cementitious Materials
(Continued)

- **References**
  - Unsaturated Zone Flow and Transport Model Process Model Report. TDR-NBS-HS-000002 Rev 00 ICN 1
  - *Drift-Scale Coupled Processes (DST and THC Seepage) Models MDL-NBS-HS-000001 Rev 00 ICN 1
  - EBS: Physical and Chemical Environment Model ANL-EBS-MD-000033 Rev 01
  - *EBS Degradation, Flow & Transport Process Model Report TDR-EBS-MD-000006 (Rev 01 is work in progress)

* Additional information to be provided in future revisions

Conclusions

- Effects of cementitious materials on performance are expected to be modest because the leachate is diluted and becomes a minor contributor to the Engineered Barrier System bulk chemical environment
- DOE considers that the NRC comment about effects of cementitious materials related to Subissue 1 has been addressed. The information presented, planned updates to the analysis/model reports and process model reports, and the additional studies being considered to confirm expectations about mountain-scale thermal-hydrological-chemical effects support a status of Closed-Pending for Subissue 1

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

Subissue 1: NRC Comments on Mineral Precipitation in Fractures or at the Fracture-Matrix Interface

Presented to:

DOE-NRC Technical Exchange on Key Technical Issue and Subissues Related to Evolution of the Near-Field Environment

Presented by:

Eric Sonnenthal
Civilian Radioactive Waste Management System Management and Operating Contractor

January 9-12, 2001
Pleasanton, CA

YUCCA MOUNTAIN PROJECT

Outline

- **Presentation Objectives**
- **Current Subissue Status**
- **For NRC comment on mineral precipitation in fractures and at the fracture-matrix interface related to Subissue 1 of the Evolution of the Near Field Environment Key Technical Issue, this presentation will**
  - Summarize technical basis for item resolution
  - Identify basis documents (References)
  - Summarize technical adequacy of basis
- **Conclusions**

Presentation Objectives

- **Provide basis for resolving NRC comments on the range of thermal-hydrological-chemical parameters associated with mineral precipitation in fractures or at the fracture-matrix interface that are related to Subissue 1**
- **DOE has developed the technical basis for neglecting mineral precipitation**
  - Near-Field Environment Process Model Report (TDR-NBS-MD-000001 Rev 00 ICN 03, Section 3.2) addresses mineral precipitation around drifts as a result of fully coupled thermal-hydrological-chemical processes
  - Unsaturated Zone Flow and Transport Process Model Report (TDR-NBS-HS-000002, Section 3.10) reviews coupled thermal-hydrological-chemical processes in the unsaturated zone around drifts
  - Engineered Barrier System Process Model Report (TDR-EBS-MD-000006 Rev 00 ICN 01, Section 3.1.2) addresses alternative models for fully coupled thermal-hydrological-chemical processes

Current Subissue Status

- Evolution of the Near-Field Environment Issue Resolution Status Report, Rev 03 indicates Subissue 1 is OPEN

Thermal-Hydrological-Chemical Parameters and Mineral Precipitation

- **NRC Comments**
  - Provide justification for the range of thermal-hydrological-chemical parameters used in the analyses
  - Modeling assumptions and choices of parameter values that affect fluid dynamics near the position of the boiling front (need for sensitivity studies)
  - Justify the treatment of fully dry fracture blocks in the TOUGHREACT reactive/transport simulations

Justification for the Range of Thermal-Hydrological-Chemical Parameters

- **Basis for Resolution**
  - DOE has performed a number of simulations of coupled thermal-hydrological-chemical processes, including sensitivity studies on the cutoff for evaluating chemistry in blocks nearing dryout conditions, and permeability-porosity coupling to mineral precipitation in fractures
  - DOE intends to evaluate the effects that alternative models have on the performance of the geologic repository

Modeling Assumptions and Choices of Parameter Values

- **Basis for Resolution**
  - Drift-Scale Coupled Processes (DST and THC Seepage) Models Analysis/Model Report (MDL-NBS-HS-000001) Rev 00 and Rev 01 (in review) used thermohydrological parameters for extrapolation of the capillary pressure as a function of liquid saturation that did not lead to fracture sealing
  - The treatment of capillary pressure at very low water saturations in fractures (much less than 1%) is uncertain. Because the treatment of fracture capillary pressures using the van Genuchten model is also uncertain, the model validation must rely on lab experiments and thermal tests
  - The parameters used are consistent with the lack of evidence of sealing in the Drift Scale Test during three years of heating

Modeling Assumptions and Choices of Parameter Values (Continued)

- **Basis for Resolution (Continued)**
  - The parameters used are also consistent with the extent of fracture-matrix interaction as evidenced by numerous water samples collected from boreholes in the Drift Scale Test and the good match to simulated results in the Drift-Scale Coupled Processes (DST and THC Seepage) Models Analysis/Model Report (MDL-NBS-HS-000001) Rev 01 (in review)
  - Sensitivity studies of the effect of changing the parameters for extrapolation on thermal-hydrological-chemical processes are expected to reduce the uncertainty in the effects of the thermal-hydrological parameters

Treatment of Fully Dry Fracture Blocks in TOUGHREACT Reactive/Transport Simulations

- The Drift-Scale Coupled Processes (DST and THC Seepage) Models Analysis/Model Report (MDL-NBS-HS-000001) Rev 01 (in review) documents simulation results of mineral precipitation using a lower saturation limit than was used in Rev 00 for performing chemical reactions (1e-5 vs. 1e-4)
- This much smaller cutoff alone has not resulted in significantly greater mineral precipitation
- The most important consideration is not necessarily the numerical technique used for treating the dryout condition (this is not unique) but that mass is conserved, which it is

Treatment of Fully Dry Fracture Blocks in TOUGHREACT Reactive/Transport Simulations (Continued)

- For any method used, such small liquid saturations are well below that required for any significant chemical effects to be important in the near-field environment
- Seepage does not occur under such conditions, and for any concentration in the fluid the greatest volume of minerals that could precipitate would be less than the volume fraction occupied by the liquid (i.e., < 1e-5)

References

- Drift-Scale Coupled Processes (DST and THC Seepage) Models Analysis/Model Report (MDL-NBS-HS-000001 Rev 01, in review)
- Unsaturated Zone Flow and Transport Model Process Model Report (TDR-NBS-HS-000002 Rev 00)
- Engineered Barrier System Degradation, Flow and Transport Process Model Report (TDR-EBS-MD-000006 Rev 00 ICN 01)
- Abstraction of Drift Scale Coupled Processes Analysis/Model Report(ANL-NBS-HS-000029 Rev 00)
- Near-Field Environment Process Model Report (TDR-NBS-MD-000001 Rev 00 ICN 03)

Conclusions

- The Drift Scale Coupled Processes (DST and THC Seepage) Models (Analysis and Model Report (MDL-NBS-HS-000001 Rev 01, in review) documents work considering alternative conceptual models and sensitivity studies of features and processes that are consistent with available data and current scientific understanding
- DOE addresses mineral precipitation around drifts as a result of fully coupled thermal-hydrological-chemical processes
- DOE has developed a technical basis for neglecting mineral precipitation in fractures and at the fracture-matrix interface

Conclusions
(Continued)

- DOE considers that this presentation, in conjunction with preceding ones, provides sufficient information to status Subissue 1 as Closed-Pending

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

Subissue 4: NRC Comments on Colloidal Transport in the Unsaturated Zone

Presented to:
DOE-NRC Technical Exchange on Key Technical Issue and Subissues Related to Evolution of the Near-Field Environment

Presented by:
Jim Houseworth
Civilian Radioactive Waste Management System Management and Operating Contractor

January 9-12, 2001
Pleasanton, CA

YUCCA MOUNTAIN PROJECT

Outline

- **Presentation Objectives**
- **Current Subissue Status**
- **For NRC comments on colloidal transport in the unsaturated zone, related to Subissue 4 of the Evolution of the Near-Field Environment Key Technical Issue, this presentation will**
  - Summarize technical basis for item resolution
  - Identify basis documents (References)
  - Summarize technical adequacy of basis
- **Conclusions**

Presentation Objectives

- Describe the basis for resolving NRC comments on colloidal transport in the unsaturated zone for Subissue 4 of the Evolution of the Near-Field Environment Key Technical Issue
- DOE has developed a model abstraction for colloid-facilitated radionuclide transport
- The abstraction is sufficient to bound the potential effects on performance because the abstraction produces a conservative estimate of the rate at which colloids move in the unsaturated zone

Current Subissue Status

- **Evolution of the Near-Field Environment Issue Resolution Status Report, Rev 03, indicates Subissue 4 is OPEN**

Colloid Transport in the Unsaturated Zone

- **NRC comments**
  - Provide additional technical bases supporting conceptual approach and detailed process models for colloid transport in the unsaturated zone
  - Provide additional technical bases for exclusions of geochemical, radiolytic, and coupled thermal-hydrological-chemical effects other than pH and ionic strength
  - Provide additional technical bases for limiting in-drift water chemistry for purposes of colloid modeling to either waste package water or a mixture of waste package water and J-13 water

[Note: The second and third comments were addressed in two earlier presentations and will not be discussed in this presentation]

Colloid Transport in the Unsaturated Zone
(Continued)

- **Basis for resolution**
  - A colloid transport model was developed to conservatively account for advection, dispersion, diffusion, radioactive decay, colloid filtration, size exclusion, and colloid-facilitated transport in the unsaturated zone
    - Colloid diffusion is conservatively set at zero
    - Size exclusion is used to keep colloids (with irreversibly attached radionuclides) in the fractures where transport rates are significantly higher
    - Filtration is limited to colloids with irreversibly attached radionuclides; credit for filtration is only taken for matrix-to-matrix transitions based on physical straining
    - Colloid retardation is conservatively neglected (retardation factor = 1)

Colloid Transport in the Unsaturated Zone
(Continued)

- **Basis for resolution (Continued)**
  - Colloids with irreversibly attached radionuclides are conserved across the Engineered Barrier System/Unsaturated Zone boundary
  - Colloids with reversibly attached radionuclides are conservatively modeled using the highest colloid concentration and K_d to define the mean value of K_c
    - Radionuclide transport facilitated by reversible association with colloids is larger (on average) in the Unsaturated Zone than in the Engineered Barrier System
    - Highest colloid concentration (C) and highest K_d (for Am on smectite) used to define a single $K_c = C \cdot K_d$ in the unsaturated zone
    - Distribution for K_c spans (4-sigma) four orders of magnitude

Colloid Transport in the Unsaturated Zone
(Continued)

- **References**
  - In-Drift Colloids and Concentration Analysis and Model Report (ANL-EBS-MD-000042 Rev 00)
  - Uncertainty Distribution for Stochastic Parameters (ANL-NBS-MD-000011 Rev 00)
  - Engineered Barrier System Degradation, Flow and Transport Process Model Report (TDR-EBS-MD-000006 Rev 00 ICN 01)
  - Unsaturated Zone Flow and Transport Process Model Report (TDR-NBS-HS-000002 Rev 00)

Conclusions

- DOE considers that the NRC comments discussed in this presentation have been adequately addressed and that this information supports a status of Closed-Pending for Subissue 4
- DOE has developed a conservative model to account for processes relevant to colloid-facilitated transport in the unsaturated zone
- DOE considers that this presentation, in conjunction with preceding ones, provides sufficient information to status Subissue 4 as Closed-Pending

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

Subissue 2: NRC Comments on In-Drift Geochemical Environment

Presented to:
DOE-NRC Technical Exchange on Key Technical Issue and Subissues Related to Evolution of the Near-Field Environment

Presented by:
Ernest Hardin
Civilian Radioactive Waste Management System Management and Operating Contractor

January 9-12, 2001
Pleasanton, CA

YUCCA MOUNTAIN PROJECT

Outline

- **Presentation Objectives**
- **Current Subissue Status**
- **For NRC comments on the in-drift geochemical environment related to Subissue 2 of the Evolution of the Near-Field Environment Key Technical Issue, this presentation will**
  - Summarize technical basis for comment resolution
  - Identify future actions which will ensure that models of the in-drift geochemical environment account for minor and trace chemical species
  - Describe integration of DOE actions to resolve the Container Life and Source Term and Evolution of the Near-Field Environment Key Technical Issues
- **Conclusions**

Presentation Objectives

- **Describe the basis for resolving NRC comments on the in-drift geochemical environment related to Subissue 2 of the Evolution of the Near-Field Environment Key Technical Issue**
- **DOE has determined**
  - Important design features are included in the Multiscale Thermo-hydrologic Model (ANL-EBS-MD-000049 Rev 00 ICN 01), which provides environmental conditions for in-drift chemical processes
  - Chemical boundary conditions (water composition, CO_2 fugacity) are provided by the Abstraction of Drift-Scale Coupled Processes (ANL-NBS-HS-000029 Rev 01 is in review), which is based on thermal-hydrologic-chemical modeling of the host rock
  - Effects from introduced materials (steel, cement) on the bulk chemical environment are addressed in the EBS physical and chemical models (e.g., ANL-EBS-MD-000033 Rev 01)

Presentation Objectives
(Continued)

- **DOE has also determined that**
  - Effects from small-scale chemical heterogeneity, dissimilar materials, and crevices on corrosion processes are addressed through the corrosion testing program
  - The in-drift chemical environment as represented in current models is consistent with corrosion test conditions
  - The inventory of introduced materials that will remain in the emplacement drifts includes elemental abundances as specified in American Society for Testing and Materials or other standards
  - Trace elements in introduced materials, or contributed by the natural system, and possible local reactions and reaction paths, will be included in ongoing and planned testing
  - The contributions of trace elements to the potential geochemical environment will be bounded using current design information, including concentrations of specified trace elements in introduced materials
  - Existing technical work and design control processes will control the incorporation of introduced material criteria into the final design basis

Current Subissue Status

- **Evolution of the Near-Field Environment Issue Resolution Status Report, Rev 03, indicates that Subissue 2 is OPEN**

In-Drift Geochemical Environment

- **NRC Comments**
  - Provide a complete description of the geochemical environment, including introduced materials and trace elements that may be important to performance
  - Calculate and/or bound the potential geochemical environments on the drip shield and waste package, considering local reactions and reaction paths
  - Document approach to complete a final design that accounts for: (a) impacts of in-drift materials on the geochemical environment and repository performance; and (b) define those materials that could be incorporated into emplacement drift area

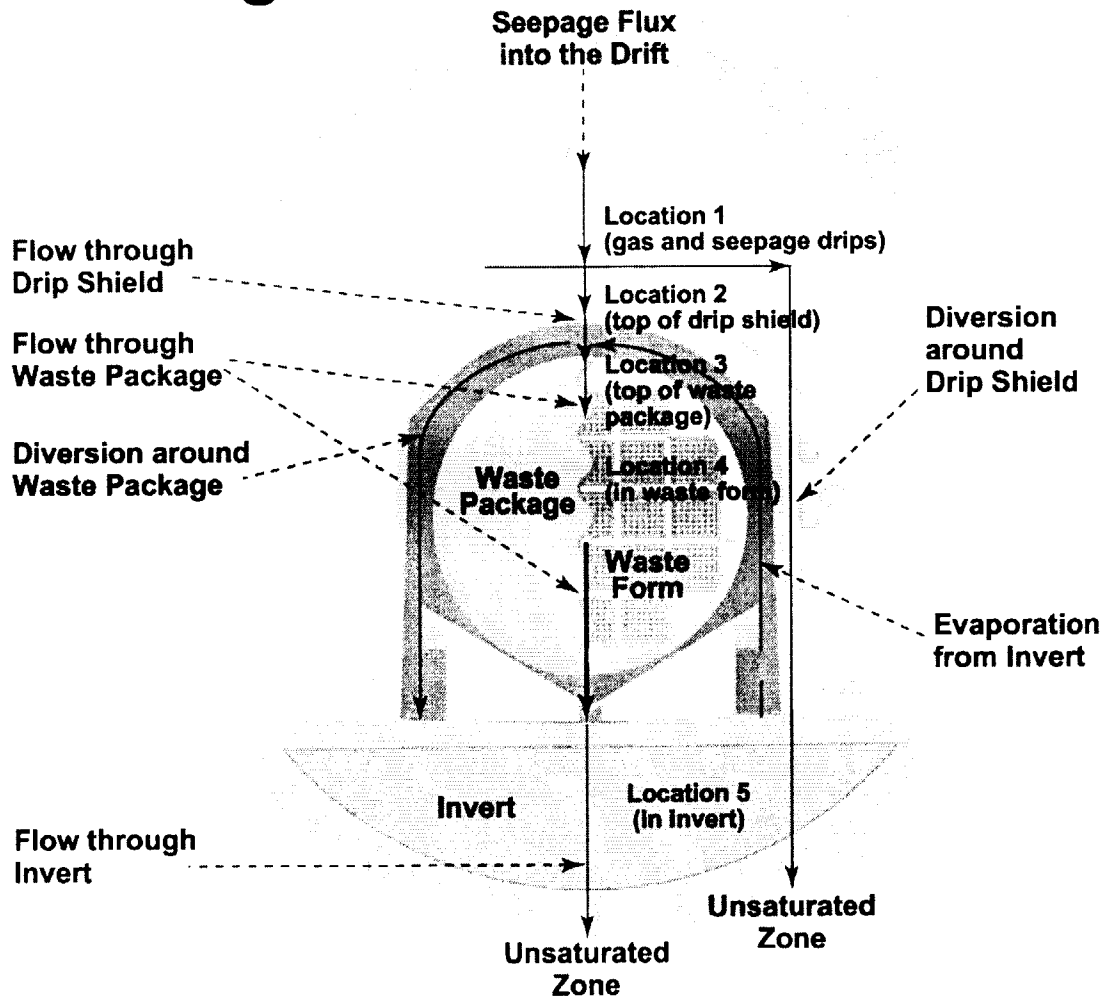
In-Drift Geochemical Environment
(Continued)

- **Basis for Resolution (Continued)**
  - The effects of evaporative concentration are included in the Precipitates/Salts Analysis modeling approach, which predicts the evolution of pH, chloride, and ionic strength
  - The potential effects of introduced materials on the bulk environment are addressed in the Engineered Barrier System: Physical and Chemical Environment Model (ANL-EBS-MD-000033 Rev 01)
  - Trace element (Pb, Hg, and As) effects on waste package and drip shield corrosion will be evaluated for resolution of the Container Life and Source Term Key Technical Issue.
  - Trace element (Pb, Hg, and As) reactions will be evaluated in updates to in-drift geochemical models

In-Drift Geochemical Environment
(Continued)

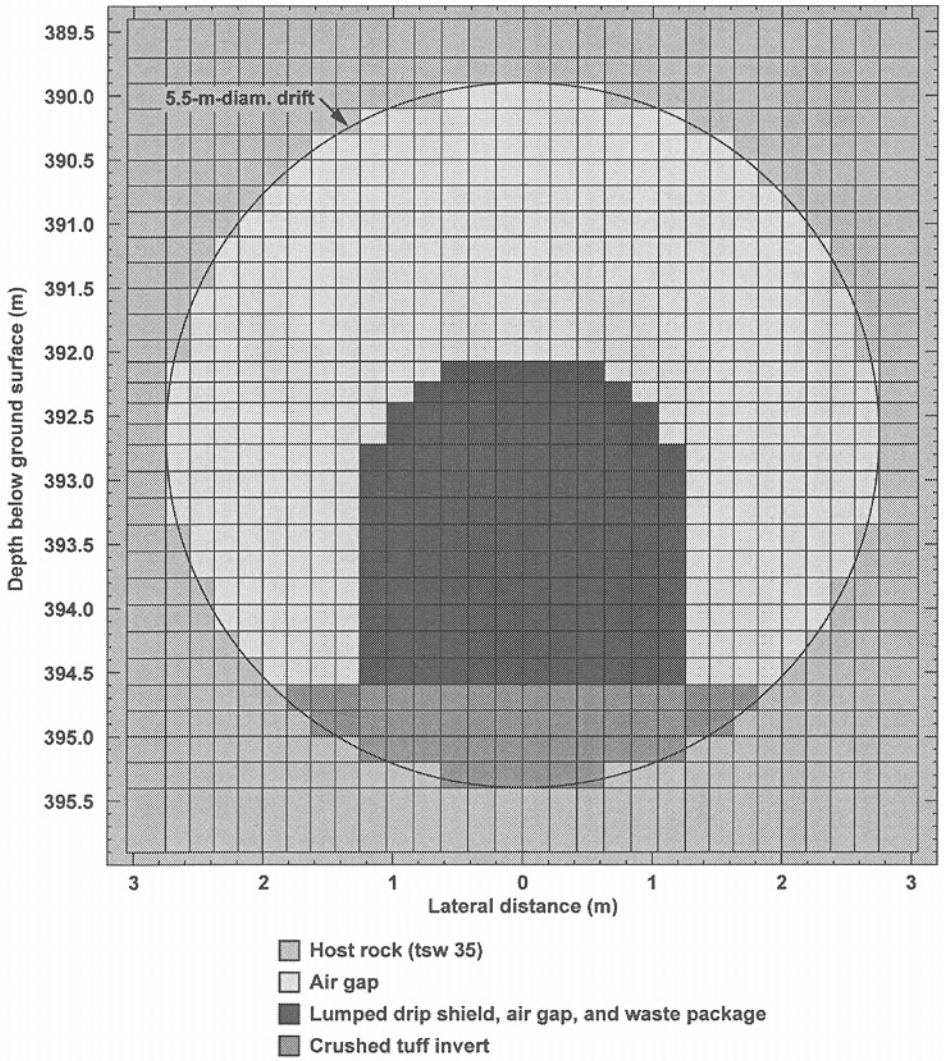
- **Basis for Resolution (Continued)**
  - Thermal-hydrologic inputs (Multiscale Thermohydrologic Model ANL-EBS-MD-000049 Rev00 ICN 01)
    - Temperature, evaporation rate
  - Thermal-hydrologic-chemical boundary conditions on the in-drift environment (Drift-Scale Coupled Processes [DST and THC Seepage] Models MDL-NBS-HS-000001 Rev 01 is in review)
    - Water composition, P_{CO2}
  - Evaporative evolution of water composition (In-Drift Precipitates/ Salts Analysis ANL-EBS-MD-000045 Rev 00 ICN 02)

In-Drift Geochemical Environment
(Continued)
Locations representing chemical environment



In-Drift Geochemical Environment
(Continued)

Model grid for two-dimensional thermo-hydrologic model (fine grid used to check model results obtained from the multiscale model)

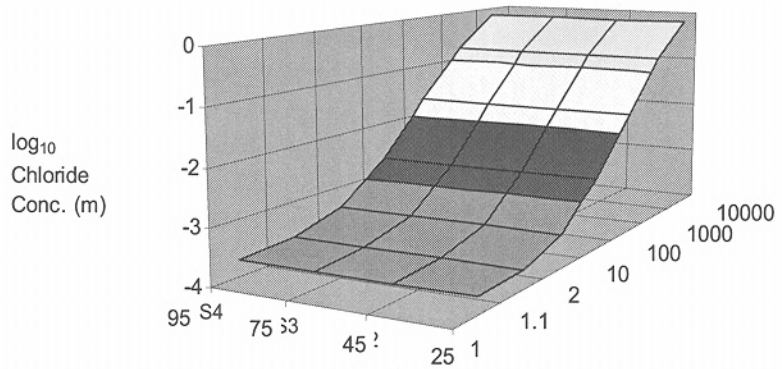


C10

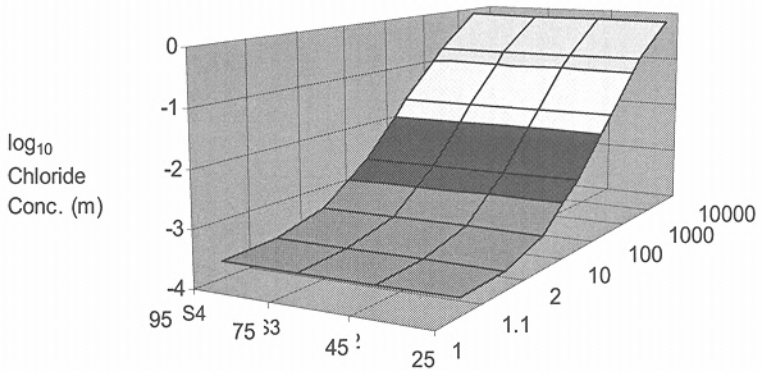
In-Drift Geochemical Environment
(Continued)

Lookup tables for chloride concentration (J-13 water calculation)

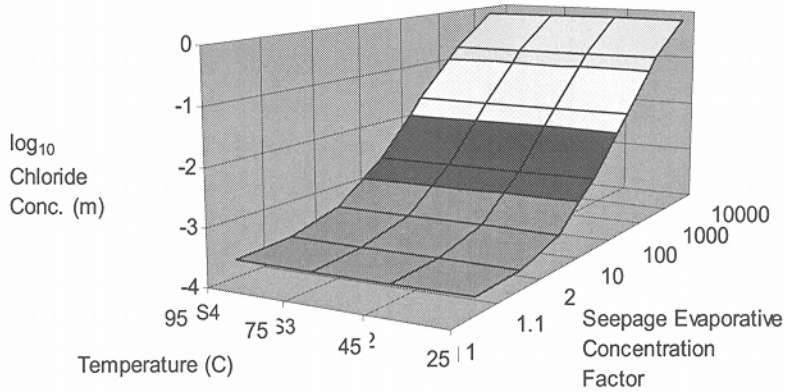
$P_{CO2} = 10^{-3}$ atm



$P_{CO2} = 10^{-1}$ atm



$P_{CO2} = 10^{-6}$ atm



Reference: In-Drift Precipitates/Salts Analysis ANL-EBS-MD-000045 Rev. 00

C11

In-Drift Geochemical Environment (Continued)

Evaporatively Concentrated Waters: Sensitivity to Starting Composition

Temperature = 96°C
Relative Humidity = 95%

Component or Property	Units	Avg. J-13 Water	Avg. Porewater	THC Seepage (Period 3)
Temperature (C)		96	96	96
Activity of water	None	0.95	0.95	0.95
$\log_{10} P_{O2}$ (redox)	None	-0.7	-0.7	-0.7
$\log_{10} P_{CO2}$	None	-6.0	-6.0	-6.5
Ionic strength	molal	2.861	1.673	1.744
pH	None	11.32	8.45	9.47
SiO2(aq)	molal	0.1378	1.363×10^{-3}	2.554×10^{-3}
Na^+	molal	2.0110	1.2557	1.5377
K^+	molal	0.1301	9.636×10^{-2}	6.320×10^{-2}
Ca^{2+}	molal	2.783×10^{-6}	0.1053	3.591×10^{-3}
Mg^{2+}	molal	2.520×10^{-8}	3.431×10^{-4}	5.110×10^{-6}
HCO_3^-	molal	0.4887	4.048×10^{-6}	3.867×10^{-5}
SO_4^{2-}	molal	0.1934	4.267×10^{-3}	0.1323
NO_3^-	molal	0.1429		
Cl^-	molal	0.2033	1.5542	1.3384
F^-	molal	0.1152	2.266×10^{-4}	9.367×10^{-4}
Li^+	molal	6.981×10^{-3}		
Sr^{2+}	molal	1.633×10^{-4}		
Fe^{2+}	molal	3.692×10^{-141}	6.288×10^{-16}	6.561×10^{-141}
Mn^{2+}	molal	1.976×10^{-20}		
Al^{3+}	molal	2.417×10^{-8}	6.873×10^{-9}	2.418×10^{-8}
HPO_4^{2-}	molal	9.547×10^{-7}		

Reference: Engineered Barrier System: Physical and Chemical Envi ronment Model ANL-EBS-MD-000033 Rev. 01

In-Drift Geochemical Environment

(Continued)

Comparison of Cement Leachate Composition with Seepage and Evaporatively Concentrated Waters

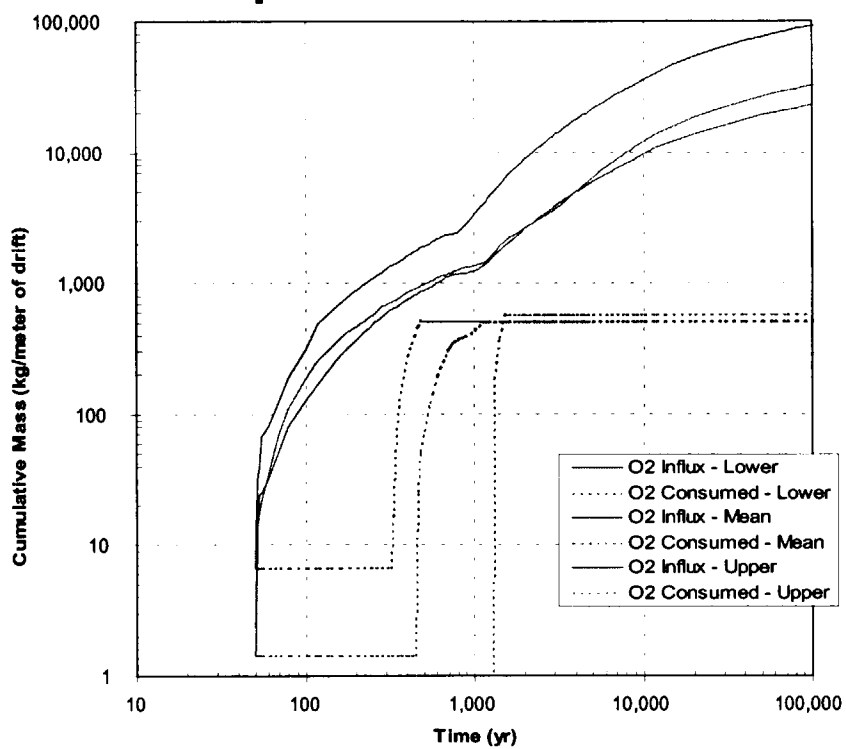
Temperature = 96°C (Period 2)

Component or Property	Units	Seepage (Period 2)	Seepage @ RH 95%	Cement Leachate	Equilibrated Leachate
Temperature (C)		96	96	96	96
$\log_{10} P_{O2}$ (redox)	None	-0.7	-0.7	-0.7	-0.7
$\log_{10} P_{CO2}$	None	-6.5	-6.5	< -6.5	-6.5
pH	None	8.1	9.5	10.3	9.2
$SiO_{2(aq)}$	molal	1.5×10^{-3}	2.554×10^{-3}	1.73×10^{-5}	1.73×10^{-5}
Na^+	molal	1.4×10^{-3}	1.5377	2.19×10^{-3}	2.19×10^{-3}
K^+	molal	8.5×10^{-5}	6.320×10^{-2}	8.50×10^{-5}	8.50×10^{-5}
Ca^{2+}	molal	6.4×10^{-4}	3.591×10^{-3}	9.62×10^{-3}	3.54×10^{-3}
Mg^{2+}	molal	3.2×10^{-7}	5.110×10^{-6}	3.54×10^{-8}	3.54×10^{-8}
HCO_3^-	molal	1.9×10^{-4}	3.867×10^{-5}	6.98×10^{-6}	1.01×10^{-5}
SO_4^{2-}	molal	6.6×10^{-4}	0.1323	3.05×10^{-3}	3.05×10^{-3}
Cl^-	molal	1.8×10^{-3}	1.3384	1.80×10^{-3}	1.80×10^{-3}
F^-	molal	2.5×10^{-5}	9.367×10^{-4}	2.50×10^{-5}	2.50×10^{-5}
Fe^{2+}	molal	7.9×10^{-10}	6.561×10^{-141}	4.58×10^{-14}	9.30×10^{-15}
Al^{3+}	molal	2.7×10^{-7}	2.418×10^{-8}	1.59×10^{-3}	5.20×10^{-4}

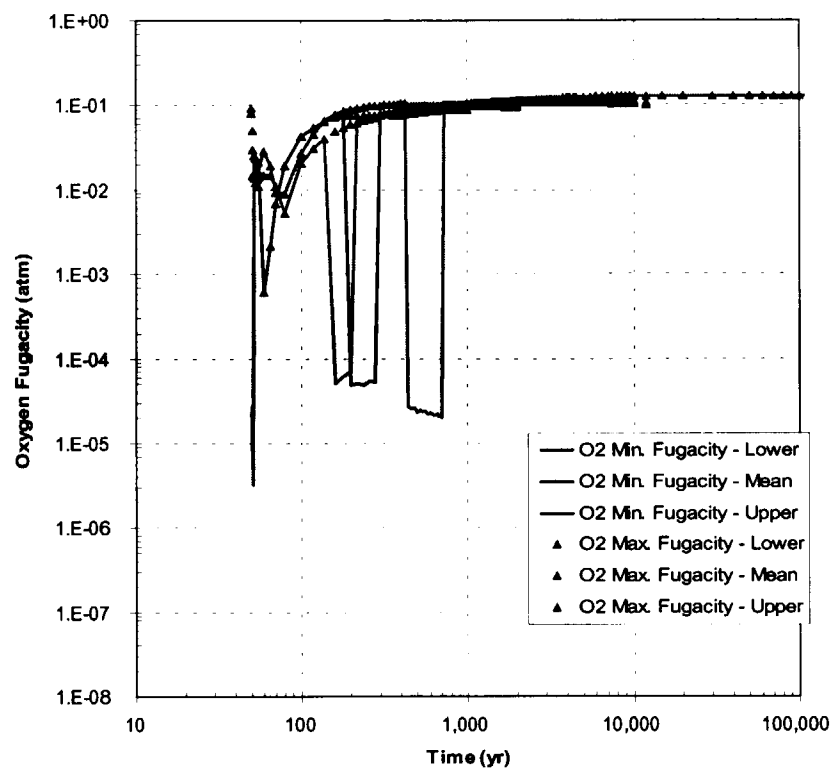
Source: Engineered Barrier System: Physical and Chemical Environ ment Model ANL-EBS-MD-000033 Rev. 01)

In-Drift Geochemical Environment
(Continued)

Cumulative O_2 Consumption by Steel Corrosion in the Emplacement Drifts



Effect of Steel Corrosion on Oxygen Fugacity



Reference: Engineered Barrier System: Physical and Chemical Environment Model ANL-EBS-MD-000033 Rev. 01)

In-Drift Geochemical Environment
(Continued)

- **Basis for Resolution, Summary**
  - DOE's current models produce expected and bounding water compositions based on behavior of major and minor chemical species
  - DOE plans to evaluate alternative reaction paths in updates to EBS geochemical models
  - DOE plans to revise the Pitzer (PT4) database and modify EQ3/6 numerical features to improve confidence in model predictions over a wider range of environmental conditions

In-Drift Geochemical Environment
(Continued)

- **References**
  - In-Drift Precipitates/Salts Analysis (ANL-EBS-MD-000045 Rev 00 ICN 02)
  - *Engineered Barrier System: Physical and Chemical Environment Model (ANL-EBS-MD-000003 Rev 01)
  - *Environments on the Surfaces of the Drip Shield and the Waste Package Outer Barrier (ANL-EBS-MD-000001 Rev 00 ICN 01)
  - *Waste Package Degradation Process Model Report (TDR-WIS-MD-000002 Rev 00 ICN 01)
  - EBS Degradation, Flow and Transport Process Model Report TDR-EBS-MD-000006 Rev 01 (work in progress)

* Additional information to be provided in future revisions

Document Approach to Complete Final Design

- **Basis for Resolution, Summary (Continued)**
  - DOE's approach to integrating and documenting design considerations uses the baseline control process (AP-3.4Q)
  - Analysis/Model Reports, Process Model Reports, and System Description Documents are baselined to ensure that performance concerns become design criteria, as appropriate

Document Approach to Complete Final Design (Continued)

- **Basis for Resolution, Summary (Continued)**
  - The potential effects of introduced materials on the bulk chemical environment are addressed in current models
  - DOE plans to evaluate Pb, Hg, and As behavior in the drift as trace species in influent waters
  - DOE plans to identify element sensitivities for corrosion-resistant materials (for both the alloys and the environment) for resolution of the Container Life and Source Term Key Technical Issue
  - DOE plans to determine potentially important trace species and limiting concentrations, prior to final specification of waste package and drip shield materials
  - DOE plans to confirm that specifications for trace metals in the Engineered Barrier System environment can be met with available materials

Document Approach to Complete Final Design (Continued)

- **References**
  - *Engineered Barrier System: Physical and Chemical Environment Model ANL-EBS-MD-000033 Rev 01
  - *Waste Package Degradation Process Model Report TDR-WIS-MD-000002 Rev 00 ICN 01
  - EBS Degradation, Flow and Transport Process Model Report TDR-EBS-MD-000006 Rev 01 (work in progress)

  * Additional information to be provided in future revisions

Conclusion

- **DOE has**
  - Included important design features in the Multiscale Thermohydrologic Model
  - Determined chemical boundary conditions for water composition and CO_2 fugacity
  - Evaluated effects of introduced materials
  - Addressed effects on corrosion of small-scale chemical heterogeneites, dissimilar materials, and crevices
  - Represented the in-drift chemical environment in current models in a manner that is consistent with corrosion test conditions
  - Planned testing and modeling to consider behavior of trace elements in the Engineered Barrier System
  - Implemented controls on the technical work and design control process that ensures incorporation of introduced material criteria into the design process

Conclusion
(Continued)

- DOE considers that NRC comments about the in-drift geochemical environment related to Subissue 2 have been addressed. The information presented and the planned additional studies to revise the Pitzer database, evaluate alternative reaction paths, evaluate the behavior of Pb, As and Hg as constituents of the natural system and engineered materials, and identify element sensitivities for corrosion resistant materials support a status of Closed-Pending for Subissue 2

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

Evolution of the Near-Field Environment Subissue 2: NRC Comments on Treatment of Coupled Processes and Model Integration

Presented to:
DOE-NRC Technical Exchange on the Evolution of the Near-Field Environment Key Technical Issue

Presented by:
Ernest Hardin
Civilian Radioactive Waste Management System
Management and Operating Contractor

January 9-12, 2001
Pleasanton, CA

YUCCA MOUNTAIN PROJECT

Outline

- **Presentation Objectives**
- **Current Subissue Status**
- **For NRC comments on the treatment of coupled processes and model integration related to Subissue 2, of the Evolution of the Near Field Environment Key Technical Issue, this presentation will**
  - Give the technical bases for the coupling strategy used for in-drift geochemical processes in current models
  - Identify specific coupling relationships that are included and excluded from Total System Performance Assessment
  - Identify improvements in integration of current models
  - Describe an alternative approach for evaluating in-drift coupled thermal-hydrological-chemical processes
- **Conclusions**

Presentation Objectives

- **Describe the basis for resolving NRC comments on the treatment of coupled processes and model integration related to Subissue 2, of the Evolution of the Near Field Environment Key Technical Issue**
- **For NRC Comments on the treatment of coupled thermal-hydrological-chemical coupled processes and model integration**
  - Coupling Relationships
    - Thermal-hydrological and thermal-chemical coupled process effects are accounted for in existing models for Total System Performance Assessment
    - Thermal-hydrological-chemical coupled process effects will be small
    - Small-scale chemical heterogeneity and transport effects are addressed in corrosion tests
    - Indirect Onsager coupled processes have been screened

Presentation Objectives
(Continued)

- **For NRC Comments on the treatment of coupled thermal-hydrological-chemical coupled processes and model integration (Continued)**
  - Alternative approach for representing thermal-hydrological-chemical coupling
    - An alternative approach is presented for evaluating in-drift coupled processes that may be important to performance, particularly inthe invert
  - Model integration
    - Models that support Total System Performance Assessment are consistent with constraints on mass and energy transport
    - Existing models that support Total System Performance Assessment use water and gas compositions based on thermal-hydrological-chemical modeling of the host rock, as boundary conditions

Current Subissue Status

- **Evolution of the Near-Field Environment Issue Resolution Status Report, Rev 03, indicates this Subissue is OPEN**

Coupling Relationships and Model Integration

- **NRC comments**
  - Stronger technical bases should be provided for the DOE's major assumption that coupled thermal-hydrological-chemical processes can be decoupled, evaluated separately, and then re-coupled without adversely affecting predictions of repository performance
  - A technical basis is required for the DOE assumption that processes, such as those described in the Gas Flux and Fugacity, Cementitious Materials, Microbial Effects, Corrosion Products, and Precipitates/ Salts models, can be treated separately without biasing predictions of how water composition will evolve over time in a complex natural and engineered environment that is subjected to a range of processes. This concern includes:
    - Insufficient integration between the DOE's various Physical and Chemical Environment models (i.e., the relationship between the water compositions used as inputs and outputs in the different process-level models)
    - The use of J-13 as an initial water composition

Coupling Relationships and Model Integration (Continued)

Organization of this presentation:

NRC Comment	Where Addressed in This Presentation
Stronger technical basis for coupling approach	Coupling Relationships Alternative Approach
Stronger technical basis for for separating submodels	Mass and Energy Fluxes
Insufficient integration	Model Integration
Use of J-13 water composition	Model Integration

Note: This presentation focuses on the coupling approach as applied to process modeling. The Total System Performance Assessment treatment of the coupling approach is discussed in the presentation by J. Nowak

Coupling Relationships Summary

- Existing models show that only minor changes in seepage magnitude and composition, and hydrological properties of the invert, will result from thermal-hydrologic-chemical coupled processes
- Separation of submodels representing in-drift processes is justified by limitations for mass and energy transfer between key locations
- Existing models for water composition in the Engineered Barrier System consider alternative water compositions and a chloride-sulfate type water (modified by thermal-hydrological-chemical processes in the host rock) is used as the influent composition

Model Integration Summary

- Existing models for water composition in the Engineered Barrier System consider alternative water compositions and a chloride-sulfate type water (modified by thermal-hydrological-chemical processes in the host rock) is used as the influent composition

Coupling Relationships Summary and Model Integration Summary (Continued)

- **The DOE considers that the NRC comments related to coupling relationships and model integration, associated with Subissue 2 have been addressed and support Closed-Pending status of Subissue 2**
- **References**
  - Engineered Barrier System Degradation, Flow and Transport Process Model Report (TDR-EBS-MD-000006 Rev 01 is work in progress)
  - *Near Field Environment Process Model Report (TDR-NBS-MD-000001 Rev 00 ICN 2)

* Additional information to be provided in future revisions

Coupling Relationships

- **Basis for Resolution**
  - Thermal-hydrological coupling relationships are included in the Multiscale Thermohydrologic Model (ANL-EBS-MD-000049 Rev 00 ICN 1)
  - Thermal effects on chemical equilibria are included in the In-Drift Precipitates/Salts Model (ANL-EBS-MD-000045 Rev 00 ICN 01)
  - Small-scale coupling relationships involving corrosion are addressed empirically by the ongoing corrosion test program documented in the Waste Package Degradation Process Model Report (TDR-WIS-MD-000002 Rev 00 ICN 01)

Coupling Relationships (Continued)

- **Basis for Resolution (Continued)**
  - Other in-drift thermal-hydrological-chemical coupled processes are negligible because
    - Production of heat and water by chemical processes is small compared to fluxes of heat and water caused by waste heat
    - Osmotic effects on thermal-hydrological processes are unimportant without evaporative concentration on the order of 1000X, representing substantial volume reduction. Associated changes in liquid fluxand other measures are therefore small compared with calculations that do not include osmotic effects
    - Osmotic effects associated with the host rock are small because seepage is limited to much less than 1 molal ionic strength
- **Reference**
    - Engineered Barrier System Degradation, Flow, and Transport Process Model Report (TDR-EBS-MD-000006 Rev 01 is work in progress)

Coupling Relationships (Continued)

- **Basis for Resolution (Continued)**
  - Onsager coupling relationships have been screened

Flux↓ Force→	**∇T**	**∇P**	$\nabla \mu$	**∇E**
Heat	**Fourier's Law**	Thermal filtration	Dufour effect	Peltier effect
Volume	Thermal osmosis	**Darcy's Law**	Chemical osmosis	Electro-osmosis
Mass	Soret effect	Reverse osmosis	**Fick's Law**	Electro-phoresis
Electric current	Seebeck effect	Streaming current	Sedimen-tation current	**Ohm's Law**

- Indirect (off-diagonal) processes are dominated by direct (main diagonal) processes for the bulk chemical environment
- Small-scale coupling relationships involving corrosion are addressed empirically by the ongoing corrosion test program

Coupling Relationships (Continued)

- **References**
  - Tsang, C.-F., and D.C. Mangold (1984). "Panel Report on Coupled Thermo-Mechanical-Hydro-Chemical Processes Associated with a Nuclear Waste Repository" (LBL-18250)
  - Engineered Barrier System Degradation, Flow and Transport Process Model Report (TDR-EBS-MD-000006 Rev 01 is work in progress)

Coupling Relationships (Continued)

- **Basis for Resolution (Continued)**
  - Specific in-drift coupling relationships have been addressed
    - Salts that can form on the metallic barriers, boiling point elevation, deliquescence, and inorganic acids as vapors (Environments on the Surface of the Drip Shield and the Waste Package Outer Barrier ANL-EBS-MD-000001 Rev 00 ICN 1)
    - Effects from contact of corroding steel with the drip shield (Hydrogen Induced Cracking of Drip Shield ANL-EBS-MD-000006 Rev 00 ICN 1)
    - Characterization of rockfall (Drift Degradation Analysis ANL-EBS-MD-000027 Rev 01)
    - Effects from rockfall on the drip shield (Design Analysis for the Ex-Container Components ANL-XCS-ME-000001 Rev 00)
    - Neutron damage to ground support (Longevity of Emplacement Drift Ground Support Materials ANL-EBS-GE-000003 Rev 01)
    - Effects from gamma radiolysis on the in-drift environment (Engineered Barrier System Degradation, Flow and Transport Process Model Report TDR-EBS-MD-000006 Rev 01 is work in progress)

Coupling Relationships - Alternative Approach

- **Basis for Resolution (Continued)**
  - Background: Current in-drift models for water composition are decoupled to represent evaporative concentration using the In-Drift Precipitates/Salts Model
  - As an alternative approach DOE plans to include the in-drift environment in the same thermal-hydrological-chemical simulations that are now used for the host rock
    - Mineral precipitates will be represented using rate laws
    - The most important results will be prediction of thermal-hydrological-chemical effects on the invert
- **References**
  - In-Drift Precipitates/Salts Analysis (ANL-EBS-MD-000045 Rev 00 ICN 01)
  - Drift-Scale Coupled Processes (DST and THC Seepage) Models (MDL-NBS-HS-000001 Rev 01 is work in progress)
  - Engineered Barrier System Degradation, Flow and Transport Process Model Report (TDR-EBS-MD-000006 Rev 01 is work in progress)

Coupling Relationships (Continued)

- **References (Continued)**
  - In-Drift Precipitates/Salts Analysis (ANL-EBS-MD-000045 Rev 00 ICN 01)
  - *EBS Physical and Chemical Environment Model (ANL-EBS-MD-000033 Rev 01)
  - Drift-Scale Coupled Processes (DST and THC Seepage) Models (MDL-NBS-HS-000001 Rev 01 is work in progress)
  - *Waste Package Degradation Process Model Report (TDR-WIS-MD-000002 Rev 00 ICN 01)
  - EBS Degradation, Flow and Transport Process Model Report (TDR-EBS-MD-000006 Rev 01 is work in progress)
  - *Near Field Environment Process Model Report (TDR-NBS-MD-000001 Rev 00 ICN 2)
  - Tsang, C.-F., and D.C. Mangold (1984). "Panel Report on Coupled Thermo-Mechanical-Hydro-Chemical Processes Associated with a Nuclear Waste Repository" (LBL-18250)
  - Hardin, E.L. and D.A. Chesnut (1997). "Synthesis Report on Thermally Driven Coupled Processes" (UCRL-ID-128495)

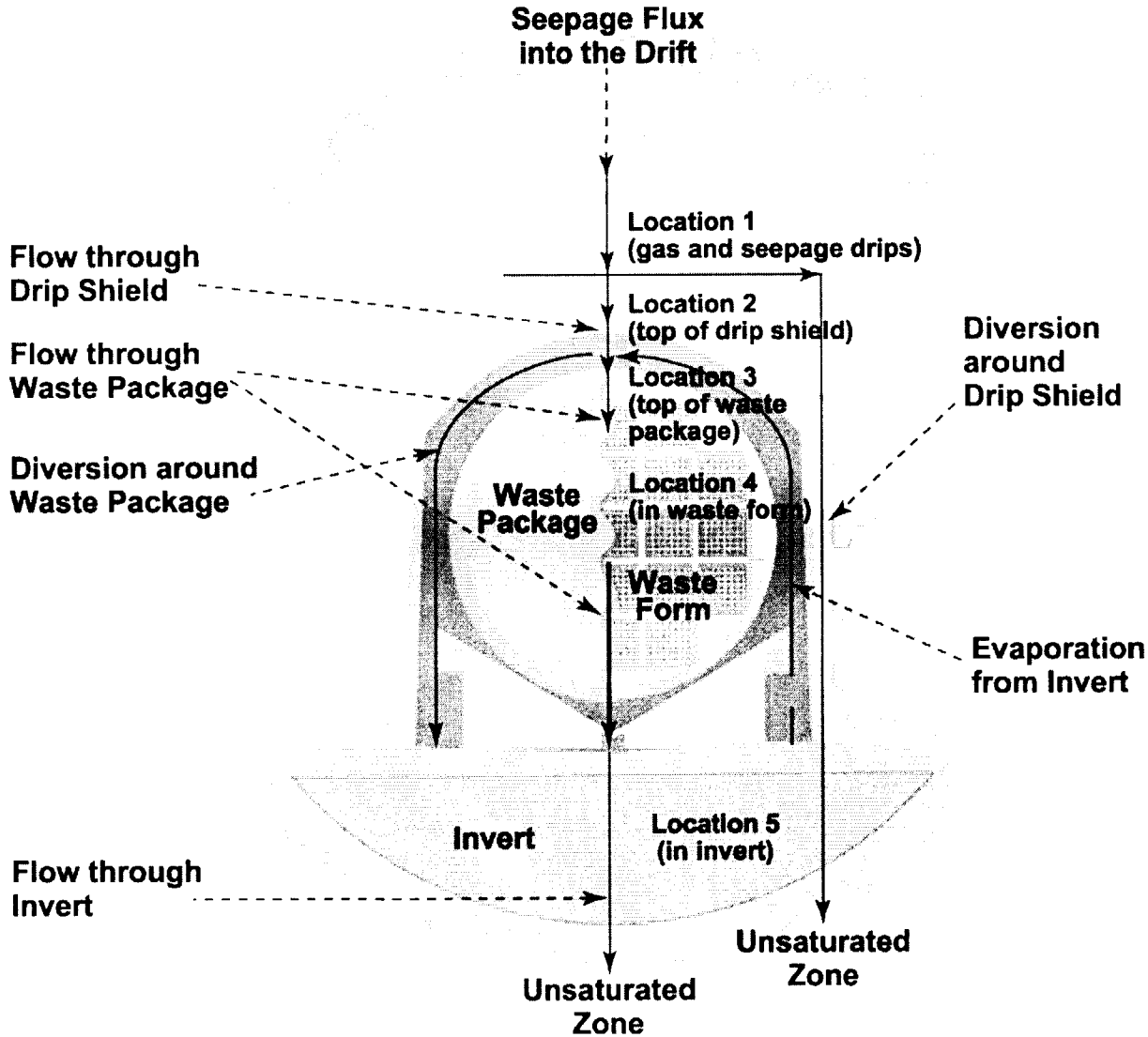
* Additional information to be provided in future revisions

Mass and Energy Fluxes

- **Basis for Resolution**
  - Processes (submodels) can be separated, simulated, and recoupled provided that important interactions are included
  - Advection, convection, and thermal radiation are the dominant modes of energy transfer and are incorporated in the Multiscale Thermohydrologic Model (ANL-EBS-MD-000049 Rev 00 ICN 1)
  - Separation of physical and chemical process submodels is justified by the separation of key locations that represent the Engineered Barrier System. Interactions between locations are unimportant if there is no solid or liquid mass transfer
  - Gas-phase composition is uniform in the Engineered Barrier System bulk environment because of mixing, and is strongly influenced by coupled processes in the host rock
  - The influence of in-drift processes on bulk gas-phase composition is minor (Engineered Barrier System Physical and Chemical Environment Model, ANL-EBS-MD-000033 Rev 01)
  - CO_2 produced by in-drift microbial processes is currently being evaluated (In-Drift Microbial Communities ANL-EBS-MD-000038 Rev 00 ICN 1)

Mass and Energy Fluxes (Continued)

- Locations representing the Engineered Barrier System



Mass and Energy Fluxes (Continued)

- **Basis for Resolution (Continued)**
  - Key locations represent the Engineered Barrier System

Location	Constituents
Rock above the drifts	Host rock, rockbolts, gas, water
1. Gas-filled space in the drifts	Dripping seepage: N_2, O_2, CO_2, H_2O
2. Surfaces of the drip shields	Water, minerals/salts, chemical transport, microbes
Gas-filled space under the drip shields	N_2, O_2, CO_2, H_2O
3. Surfaces of the waste packages	Water, minerals/salts, chemical transport, microbes
Inner surfaces of the waste packages	Water, minerals/salts, chemical transport
4. Waste form	Water, minerals/salts, radionuclide transport
5. Invert below the waste packages	Water, minerals/salts, radionuclide transport, microbes

  - Gas-phase composition is uniform at all locations except inside the waste package
  - Models that support Total System Performance Assessment are consistent with *downward* liquid or solid transport

Mass and Energy Fluxes (Continued)

- **Basis for Resolution (Continued)**
  - Current models implemented in Total System Performance Assessment represent important mass and energy transfer relationships among the locations representing the Engineered Barrier System
  - Corrosion tests directly investigate small-scale chemical interaction in crevices, and at contacts between dissimilar materials including steel
  - Gas phase transport/coupling via oxygen and carbon dioxide has been considered

Mass and Energy Fluxes (Continued)

- **References**
  - *Engineered Barrier System: Physical and Chemical Environment Model (ANL-EBS-MD-000033 Rev 01)
  - *Physical and Chemical Environment Abstraction Model (ANL-EBS-MD-000046 Rev 00 ICN 1)
  - Engineered Barrier System Degradation, Flow and Transport Process Model Report (TDR-EBS-MD-000006 Rev 01 is work in progress)
  - Hydrogen Induced Cracking of Drip Shield (ANL-EBS-MD-000006 Rev 00 ICN 1)
  - *Drift Degradation Analysis (ANL-EBS-MD-000027 Rev 01)
  - *Design Analysis for the Ex-Container Components (ANL-XCS-ME-000001 Rev 00)
  - Longevity of Emplacement Drift Ground Support Materials (ANL-EBS-GE-000003 Rev 01)

  * Additional information to be provided in future revisions

Model Integration

- **Basis for Resolution**
  - Current models use abstracted water compositions from thermal-hydrological-chemical modeling of the host rock, as the drift-wall boundary condition for the in-drift geochemical environment (thus, the representation of water composition is consistent and integrated)
  - The type of water represented by the thermal-hydrological-chemical model results (chloride-sulfate type) has been incorporated in corrosion testing

Model Integration (Continued)

- **References**
  - *Engineered Barrier System: Physical and Chemical Environment Model (ANL-EBS-MD-000033 Rev 01)
  - *Physical and Chemical Environment Abstraction Model (ANL-EBS-MD-000046 Rev 00 ICN 1)
  - *Environments on the Surfaces of the Drip Shield and Waste Package Outer Barrier (ANL-EBS-MD-000001 Rev 00 ICN 1)
  - Engineered Barrier System Degradation, Flow and Transport Process Model Report (TDR-EBS-MD-000006 Rev 01 is work in progress)
  - *Waste Package Degradation Process Model Report (TDR-WIS-MD-000002 Rev 00 ICN 01)

  * Additional information to be provided in future revisions

Conclusions

- Thermal-hydrological coupling and thermal effects on chemical equilibrium are included in current models that support Total System Performance Assessment
- Thermal-hydrological-chemical coupled process effects will be small
- Small-scale chemical heterogeneity and transport effects are addressed in corrosion tests
- Indirect Onsager coupled processes have been screened
- An alternative approach will be used to evaluated thermal-hydrological-chemical processes in the Engineered Barrier System, particularly for the invert
- Separation of submodels is justified based on in -drift mass and energy transfer relationships

Conclusions (Continued)

- Models that support Total System Performance Assessment are consistent with constraints on mass and energy transport
- Existing models that support Total System Performance Assessment use water and gas compositions based on thermal-hydrological-chemical modeling of the host rock, as boundary conditions
- DOE considers the NRC comments on coupling relationships and model integration, associated with Subissue 2, have been addressed. The information presented and planned additional studies to update analysis/model reports and process model reports and evaluate the alternative approach support a status of Closed-Pending for Subissue 2

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

Subissue 2, NRC Comments on the Assumption of Chemical Equilibrium

Presented to:
DOE-NRC Technical Exchange on Key Technical Issue and Subissues Related to Evolution of the Near-Field Environment

Presented by:
Ernest Hardin
Tom Wolery
Civilian Radioactive Waste Management System Management and Operating Contractor

January 9-12, 2001
Pleasanton, CA

YUCCA MOUNTAIN PROJECT

Outline

- **Presentation Objectives**
- **Current Subissue Status**
- **For NRC comments about the assumption of chemical equilibrium related to Subissue 2 of the Evolution of the Near Field Environment Key Technical Issue, this presentation will**
  - Provide the technical bases justifying the assumption of chemical equilibrium
  - Identify the Analysis Model Reports and Process Model Reports that use the equilibrium assumption and that will provide additional support in planned revisions
  - Identify the Analysis Model Reports and Process Model Reports in which planned reactive transport modeling of the Engineered Barrier System will be documented
- **Conclusions**

Presentation Objectives

- **Describe the basis for resolving NRC comments about the assumption of chemical equilibrium related to Subissue 2 of the Evolution of the Near Field Environment Key Technical Issue**
- **DOE has determined**
  - Current models are consistent with laboratory data (e.g., apparent fluorite precipitation in evaporation tests)
  - Current models are consistent with mineral paragenetic relationships from site characterization (e.g., calcite reactivity)
  - Multiple mineral species are available as possible precipitates for particular chemical components (e.g., sellaite)
  - Sensitivity of model results for bulk chemistry will be assessed by suppressing and/or substituting mineral precipitates
  - Reactive transport will be used for comparison to models that assume mineral equilibrium

Current Subissue Status

- **Evolution of the Near-Field Environment Issue Resolution Status Report, Rev 03, indicates Subissue 2 is OPEN**

Chemical Equilibrium

- **NRC comment**
  - Stronger technical bases should be provided for the DOE's major assumption that all reactions proceed to equilibrium. The suppression of mineral precipitation in EQ3/6 calculations, as in the Precipitates/Salts AMR, is an acknowledgement of the role of kinetics

Chemical Equilibrium
(Continued)

- **Basis for Resolution**
  - The In-Drift Precipitates/Salts Analysis/Model Report (ANL-EBS-MD-000045 Rev 00 ICN 02) assumes equilibrium to calculate pH, ionic strength, and chloride concentration for waters in the Engineered Barrier System
  - Equilibrium solids used in these models are consistent with laboratory observations
    - Halite, gypsum (or anhydrite), and silica are principal precipitates
    - Other minor minerals (totaling <10% of predicted precipitates in moles) that were observed or inferred from laboratory tests include fluorite, clays, and tachyhydrite

Chemical Equilibrium
(Continued)

- **Basis for Resolution (Continued)**
  - Current models are consistent with laboratory data
  - Precipitates selected/suppressed in current models are consistent with known paragenetic relationships (e.g. occurrence of calcite in fractures in the host rock)

Chemical Equilibrium
(Continued)

Mineralogical Results from Test with Synthetic Porewater (evap3)

evap3—1243×	evap3—Complete Evaporation
gypsum ($CaSO_4{:}2H_2O$)	gypsum ($CaSO_4{:}2H_2O$) tachyhydrite ($CaMg_2Cl_6O_{10}{:}12H_2O$)

Source: DTN: LL991008004241.041

Mineralogic Results from Test with Synthetic Porewater and Tuff (evap5)

evap6—564×	evap6—Complete Evaporation [A]
gypsum ($CaSO_4{:}2H_2O$) halite (NaCl)	gypsum ($CaSO_4{:}2H_2O$) halite (NaCl) Mg-smectite ($Na_{.3}(Al,Mg)_2Si_4O_{10}(OH)_2$) Kenyaite ($NaSi_{11}O_{20.5}(OH)_4{:}3\ H_2O$)[B]

Source: EBS Physical and Chemical Environment Model Analysis/Model Report (ANL-EBS-MD-000033 Rev. 01)

NOTES: A Only the minerals produced by evaporation and not present in the starting tuff are reported here. The major minerals constituting the tuff are probably crystobalite (α), K-feldspar, albite, anorthite, and quartz.

B Species is a minor constituent and identification is uncertain.

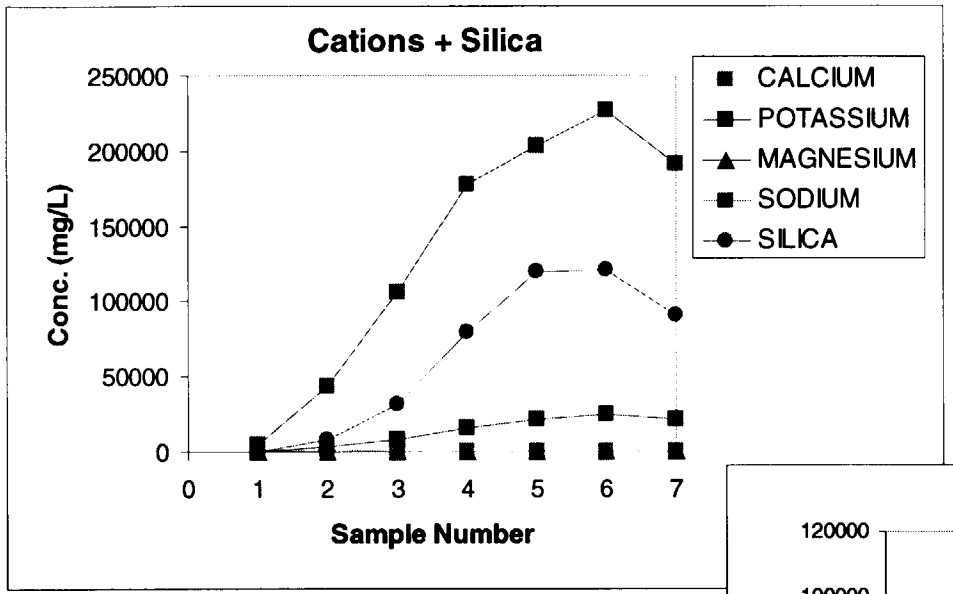
Chemical Equilibrium
(Continued)

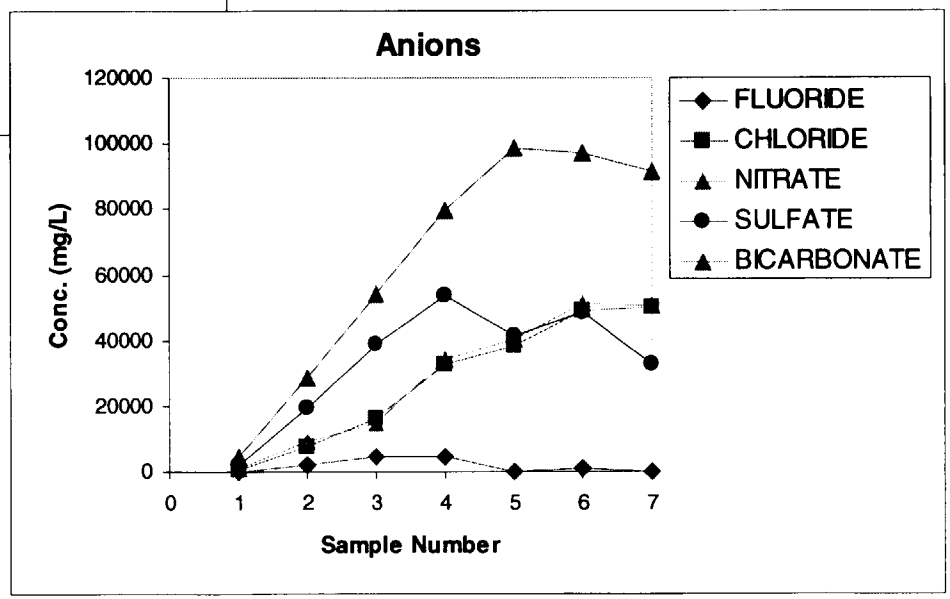
Normative Model for Precipitates Formed from Evaporating 1 kg of Synthetic Porewater, Compared with Laboratory Qualitative Observations

Predicted Normative Species	Predicted Moles/kg	Detected Species
Species Constituting >90% of Total Molality		
Gypsum/anhydrite ($CaSO_4$)	8.734E–04	Gypsum ($CaSO_4{:}2H_2O$)
Tachyhydrite ($CaMg_2Cl_6O_{10}{:}12H_2O$)	2.427E–04	Tachyhydrite ($CaMg_2Cl_6O_{10}{:}12H_2O$)
Silica (amorphous)	3.702E–04	
Calcite ($CaCO_3$)	2.567E–04	
Halite (NaCl)	3.021E–04	
Remaining Species		
Niter (KNO_3)	1.023E–04	
Na-niter ($NaNO_3$)	7.025E–05	
Fluorite (CaF_2)	5.684E–05	

Source: EBS Physical and Chemical Environment Model Analysis/Model Report (ANL-EBS-MD-000033 Rev. 01)

Evaporation of Simulated J-13
Near-Boiling Temp. and RH 85%





Source:
Environments on the Surfaces of the Drip Shield and Waste Package Outer Barrier (ANL-EBS-MD-000001 Rev. 00 ICN 01)

Comparison of Results from Evaporation Tests to Precipitates/Salts Model Predictions

Component (Concentrations are molal except pH)	Evaporation of Synthetic Average J-13 Well Water at 85°C (Concentration factor: 157)		Evaporation of Synthetic 100x Average J-13 Well Water at 90°C and 85% Relative Humidity (Effective concentration factor: 2,070)		Evaporation of Synthetic Topopah Spring Tuff Pore Water at 75°C (Concentration factor: 1,243)	
	Experimental Results	Model Predictions	Experimental Results	Model Predictions	Experimental Results	Model Predictions
pH	10.18	9.90	not reported	10.03	6.25	6.50
Ionic strength	2.45E-01	4.43E-01	3.60E+00	3.69E+00	2.79E+00	4.81E+00
Na	2.30E-01	3.07E-01	3.32E+00	3.44E+00	2.59E-01	4.33E-01
K	1.43E-02	1.95E-02	2.77E-01	2.48E-01	7.11E-02	1.30E-01
Ca	2.99E-05	1.42E-06	8.98E-04	1.75E-06	3.90E-01	5.50E-01
Mg	2.06E-06	1.84E-08	0.00E-00 [A]	2.16E-06	2.25E-01	5.12E-01
Cl	2.39E-02	3.29E-02	4.07E-01	3.87E-01	1.50E+00	2.67E+00
CO_3	7.04E-02	1.11E-01	8.95E-01	1.15E+00	< 5.74E-04 [B]	4.56E-05
SO_4	2.25E-02	3.08E-02	3.10E-01	3.19E-01	2.16E-02	6.14E-03
SiO_2	1.66E-02	2.82E-03	not included in test		8.54E-03	4.82E-04
F	1.30E-02	1.97E-02	1.91E-01	1.97E-01	< 3.04E-02 [B]	1.53E-03
NO_3	1.69E-02	2.01E-02	2.27E-01	2.22E-01	not measured	2.15E-01

NOTES:

A. Zero concentration reported; no detection limit available

B. Below detection limit

Reference: In-Drift Precipates/Salts Analysis ANL-EBS-MD-000045, Rev 00, ICN 02

Chemical Equilibrium
(Continued)

- **Basis for Resolution (Continued)**
  - **Multiple mineral species are available as possible precipitates**
    - Alternative mineral precipitates are in the chemical database, and some have been considered (e.g. sellaite for fluorite). Work in progress will further evaluate the sensitivity of calculated results and will include reaction path modeling (EQ6) where appropriate

Chemical Equilibrium
(Continued)

- **Basis for Resolution (Continued)**
  - **Reactive transport (alternative approach)**
    - The THC seepage model uses an alternative, kinetically based approach. Planned work will modify this model to incorporate in-drift processes, to evaluate consistency between models (i.e., to compare results obtained for the Drift-Scale Coupled Processes [DST and THC Seepage] Model, and the Engineered Barrier System Physical and Chemical Environment Model)

Chemical Equilibrium
(Continued)

- **Technical Basis for Closure (Continued)**
  - References
    - In-Drift Precipitates/Salts Analysis (ANL-EBS-MD-000045 Rev 00 ICN 01)
    - *EBS Physical and Chemical Environment Model (ANL-EBS-MD-000033 Rev 01)
    - *Drift-Scale Coupled Processes (DST and THC Seepage) Models (MDL-NBS-HS-000001 Rev 01)
    - EBS Degradation, Flow and Transport PMR (TDR-EBS-MD-000006 Rev 01 is work in progress)
    - Near Field Environment PMR (TDR-NBS-MD-000001 Rev 01 is work in progress)
    - Unsaturated Zone Flow and Transport Model PMR (TDR-NBS-HS-000002 Rev 01 is work in progress)

* Additional information to be provided in future revisions

Conclusions

- DOE considers that the NRC comments about the assumption of chemical equilibrium have been addressed. The information presented and planned additional studies to update analysis/model reports support a status of Closed-Pending for Subissue 2
- The chemical equilibrium assumption used in current analysis/model reports and process model reports is justified based on comparison with laboratory test results and paragenetic relationships
- DOE considers that this presentation, in conjunction with preceding ones, provides sufficient information to status Subissue 2 as Closed-Pending

Backup Slides

Period 3 THC-seepage water modified to RH = 90% at T = 90°C
Effect on water composition of suppressing minerals in the base set

Mineral Suppressed	Initial PWS3 Water	None	Clino-hy-Na	Calcite	Anhydrite	Cristobalite(α)	Fluorite
RH @ 90 C		0.90	0.90	0.90	0.90	0.90	0.90
pH		7.74	7.74	9.35	6.58	7.76	7.73
I (molal)		3.46	3.46	3.46	4.95	2.37	3.42
Evap.Conc.		786	786	788	650	543	783
Solute Dissolved Inventory (moles)							
Al	6.80E-08	3.10E-12	6.79E-08	3.01E-12	4.68E-12	3.72E-25	3.26E-12
C	3.00E-04	8.99E-07	8.99E-07	1.86E-04	6.06E-08	1.34E-06	8.73E-07
Ca	1.00E-03	2.95E-06	2.95E-06	8.49E-06	8.06E-04	4.59E-06	3.62E-06
Cl	3.20E-03	3.20E-03	3.20E-03	3.20E-03	3.20E-03	3.20E-03	3.20E-03
F	4.50E-05	1.37E-06	1.37E-06	1.04E-06	4.16E-07	2.08E-06	4.50E-05
K	3.10E-04	3.10E-04	3.10E-04	3.10E-04	3.10E-04	3.10E-04	3.10E-04
Mg	1.60E-06	1.60E-06	1.60E-06	1.60E-06	1.60E-06	1.60E-06	1.60E-06
Na	3.68E-03	3.68E-03	3.68E-03	3.68E-03	3.68E-03	3.68E-03	3.68E-03
S	1.20E-03	3.96E-04	3.96E-04	2.30E-04	1.20E-03	3.66E-04	3.75E-04
Si	2.10E-03	7.88E-07	7.88E-07	2.03E-06	9.64E-07	2.10E-03	7.98E-07
Solids Inventory (moles)							
Clinoptilolite-hy-Na		1.97E-08	0	1.97E-08	1.97E-08	1.97E-08	1.97E-08
Calcite		1.72E-04	1.72E-04	0	1.72E-04	1.40E-04	1.72E-04
Nontronite-Na		3.75E-11	2.05E-10	3.75E-11	3.75E-11	3.75E-11	3.75E-11
Cristobalite(alpha)		2.10E-03	2.10E-03	2.10E-03	2.10E-03	0	2.10E-03
Anhydrite		8.04E-04	8.04E-04	9.70E-04	0	8.34E-04	8.25E-04
Fluorite (CaF_2)		2.18E-05	2.18E-05	2.20E-05	2.23E-05	2.15E-05	0
Precipitated as a Fraction of Total:							
Al as Clinoptilolite-hy-Na (Al 3.45)		1.00E+00	0	1.00E+00	1.00E+00	1.00E+00	1.00E+00
Ca as Calcite		1.72E-01	1.72E-01	0	1.72E-01	1.40E-01	1.72E-01
S as Anhydrite		6.70E-01	8.04E-01	9.70E-01	0	8.34E-01	8.25E-01
Si as Cristobalite(α)		9.99E-01	1.00E+00	9.99E-01	9.99E-01	0	9.99E-01
F as Fluorite		4.85E-01	4.85E-01	4.88E-01	4.95E-01	4.77E-01	0

Reference: EBS Physical and Chemical Environment AMR Rev 01; work in progress

Effect on water composition of suppressing minerals in the base set

J-13 water modified to RH = 90% at T = 90°C

Mineral Suppressed	Initial J-13 Water	None	Calcite	Analcime	Brucite	Sellaite
Temp.(C)	25	90	90	90	90	90
pH		9.83	9.65	9.83	9.81	9.81
I (molal)		6.74	8.89	6.74	7.02	6.44
Evap.Conc.		2260	2055	2260	2270	2190
Solute Dissolved Inventory (moles)						
Al	2.12E-10	4.10E-12	3.65E-12	2.11E-10	3.93E-12	4.25E-12
C	2.18E-03	7.11E-04	1.06E-03	7.11E-04	7.49E-04	6.66E-04
Ca	3.67E-04	1.68E-09	3.67E-04	1.68E-09	1.72E-09	1.83E-09
Cl	2.01E-04	2.01E-04	2.01E-04	2.01E-04	2.01E-04	2.01E-04
F	1.15E-04	2.54E-05	3.34E-05	2.54E-05	6.48E-07	1.15E-04
K	1.29E-04	1.29E-04	1.29E-04	1.29E-04	1.29E-04	1.29E-04
Li	6.92E-06	6.92E-06	6.92E-06	6.92E-06	6.92E-06	6.92E-06
Mg	8.27E-05	1.52E-08	2.83E-08	1.52E-08	2.56E-05	1.71E-08
Mn	1.81E-16	1.48E-20	2.72E-20	1.48E-20	1.54E-20	1.52E-20
N	1.42E-04	1.42E-04	1.42E-04	1.42E-04	1.42E-04	1.42E-04
Na	1.99E-03	1.99E-03	1.99E-03	1.99E-03	1.99E-03	1.99E-03
S	1.92E-04	1.92E-04	1.92E-04	1.92E-04	1.92E-04	1.92E-04
Si	1.01E-03	1.61E-06	1.30E-06	1.61E-06	1.53E-06	1.60E-06
Sr	4.57E-07	4.57E-07	4.57E-07	4.57E-07	4.57E-07	4.57E-07
Solids Inventory (moles)						
Clinoptilolite-hy-Na		4.28E-13	4.28E-13	4.28E-13	4.28E-13	4.28E-13
Calcite		3.67E-04	0	3.67E-04	3.67E-04	3.67E-04
Analcime		2.15E-10	2.16E-10	0	2.16E-10	2.15E-10
Cristobalite(alpha)		1.01E-03	1.01E-03	1.01E-03	1.01E-03	1.01E-03
Brucite		3.80E-05	4.20E-05	3.80E-05	0	8.27E-05
Pyrolusite		1.81E-16	1.81E-16	1.81E-16	1.81E-16	1.81E-16
Sellaite (MgF_2)		4.47E-05	4.07E-05	4.47E-05	5.70E-05	0
Precipitated as a Fraction of Total:						
Al as Analcime (Al 0.96)		9.74E-01	9.76E-01	0.00E+00	9.75E-01	9.73E-01
Ca as Calcite		1.00E+00	0.00E+00	1.00E+00	1.00E+00	1.00E+00
Si as Cristobalite(α)		9.98E-01	9.99E-01	9.98E-01	9.98E-01	9.98E-01
F as Sellaite (MgF_2)		3.89E-01	3.54E-01	3.89E-01	4.97E-01	0.00E+00

Reference: EBS Physical and Chemical Environment AMR Rev 01; work in progress

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

Subissue 2: Range of Water Chemistry and Trace Elements in the Waste Package Chemical Environment

Presented to:
DOE-NRC Technical Exchange on Key Technical Issue and Subissues Related to Evolution of the Near-Field Environment

Presented by:
Gregory Gdowski
Civilian Radioactive Waste Management System Management and Operating Contractor

January 9-12, 2001
Pleasanton, CA

YUCCA MOUNTAIN PROJECT

Outline

- **Presentation Objectives**
- **Current Subissue Status**
- **For NRC comments on the range of water chemistry and trace elements related to Subissue 2 of the Evolution of the Near-Field Environment Key Technical Issue, this presentation will**
  - Describe the range of water chemistry in the waste package chemical environment
  - Identify analysis/model reports and process model reports that support the range of water chemistry and which will provide additional support in planned revisions
- **Conclusions**

Presentation Objectives

- Describe the basis for resolving NRC comments on the waste package chemical environment related to Subissue 2 of the Evolution of the Near-Field Environment Key Technical Issue
- DOE has collected information needed to develop models of the waste package chemical environment and for corrosion testing of candidate materials for the drip shield and waste package outer barrier
- Trace elements are being addressed in ongoing work
- The performance of the titanium drip shield is part of the corrosion test program which considers the implications of fluoride concentration

Current Subissue Status

- Evolution of the Near Field Environment Issue Resolution Status Report, Rev 03, indicates Subissue 2 is OPEN

Range of Water Chemistry and Trace Elements

- **NRC comments**
  - Provide information on the range of water chemistry that could evolve in the potential repository, including trace metals that could influence drip shield and waste package performance. This information is used to define the geochemical environment in the various conceptual models and define aqueous solutions for corrosion testing of candidate materials. Measurement of trace elements in thermal (field study) waters and laboratory waters will be measured to the extent possible
  - Provide additional laboratory and/or field data on the performance of the titanium drip shield, especially in the presence of fluoride containing solutions

Range of Water Chemistry

- **Basis for Resolution**
  - Five processes have been identified and addressed in existing models as controlling the chemistry of water contacting the waste packages:
    - Seepage of water and its flow within the drift
    - Evaporation and condensation
    - Deposition of salts and precipitates within the drift
    - Chemical reactions between water, rock, and introduced materials
    - Accumulation of corrosion products within the drifts and their effect on chemistry and flow

Range of Water Chemistry
(Continued)

- **References**
  - *Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier (ANL-EBS-MD-000001 Rev 00)
  - In-Drift Precipitates/Salts Analysis (ANL-EBS-MD-000045 Rev 00 ICN 02)
  - *Physical and Chemical Environment Abstraction Model (ANL-EBS-MD-000046 Rev 00 ICN 01)
  - *Engineered Barrier System Physical and Chemical Environment Model (ANL-EBS-MD-000033 Rev 01)
  - *Drift-Scale Coupled Processes (DST and THC Seepage) Models (MDL-NBS-HS-000001 Rev 01, is in review)
  - *Waste Package Degradation Process Model Report (TDR-WIS-MD-000002 Rev 00 ICN 01)

*Additional information is to be provided in future revisions

Range of Water Chemistry
(Continued)

- **References (Continued)**
  - *EBS Degradation, Flow and Transport Process Model Report (TDR-EBS-MD-000006 Rev 01 work in progress)
  - Near Field Environment Process Model Report (TDR-NBS-MD-000001 Rev 01 work in progress)

*Additional information is to be provided in future revisions

Range of Water Chemistry
(Continued)

- **Basis for Resolution (Continued)**
  - DOE has performed studies to characterize the brines that will form on the drip shield and waste package outer barrier from dilute Yucca Mountain waters. These studies have included
    - Analyses of dissolved trace elements
    - Evaporative concentration of waters
    - Evaporative concentration of chloride-sulfate-type and bicarbonate-type waters
    - Effects of introduced materials on water chemistry
  - Additional studies are planned to extend the water chemistry database and collect confirmatory information

Range of Water Chemistry
(Continued)

- **References (Continued)**
  - *Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier (ANL-EBS-MD-000001 Rev 00)
  - *EBS Physical and Chemical Environment Model (ANL-EBS-MD-000033 Rev 01)

*Additional information is to be provided in future revisions

Range of Water Chemistry
(Continued)

- **Basis for Resolution (Continued)**
  - DOE has analyzed a wide range of different waters
  - DOE has analyzed waters from thermal tests in the Exploratory Studies Facility
    - Drift Scale Test water
    - Single Heater Test water
  - DOE has analyzed laboratory aqueous solutions
    - Evaporatively concentrated waters from laboratory tests
    - Waters from wetting of mineral/salt precipitates in laboratory evaporative tests
    - Aqueous solutions used for long-term corrosion tests
  - DOE plans to analyze laboratory solutions that have interacted with introduced materials

Range of Water Chemistry
(Continued)

- **Basis for Resolution (Continued)**
  - Water compositions used for Total System Performance Assessment are abstracted from the Drift-Scale Coupled Processes (DST and THC Seepage) Models (MDL-NBS-HS-000001 Rev 01, is in review). This model uses a chloride-sulfate type water composition as the far-field boundary condition

Range of Water Chemistry
(Continued)

- **References**
  - *Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier (ANL-EBS-MD-000001 Rev 00)
  - *EBS Physical and Chemical Environment Model (ANL-EBS-MD-000033 Rev 01)
  - *Drift-Scale Coupled Processes (DST and THC Seepage) Models (MDL-NBS-HS-000001 Rev 01, is in review)

*Additional information is to be provided in future revisions

Range of Water Chemistry
(Continued)

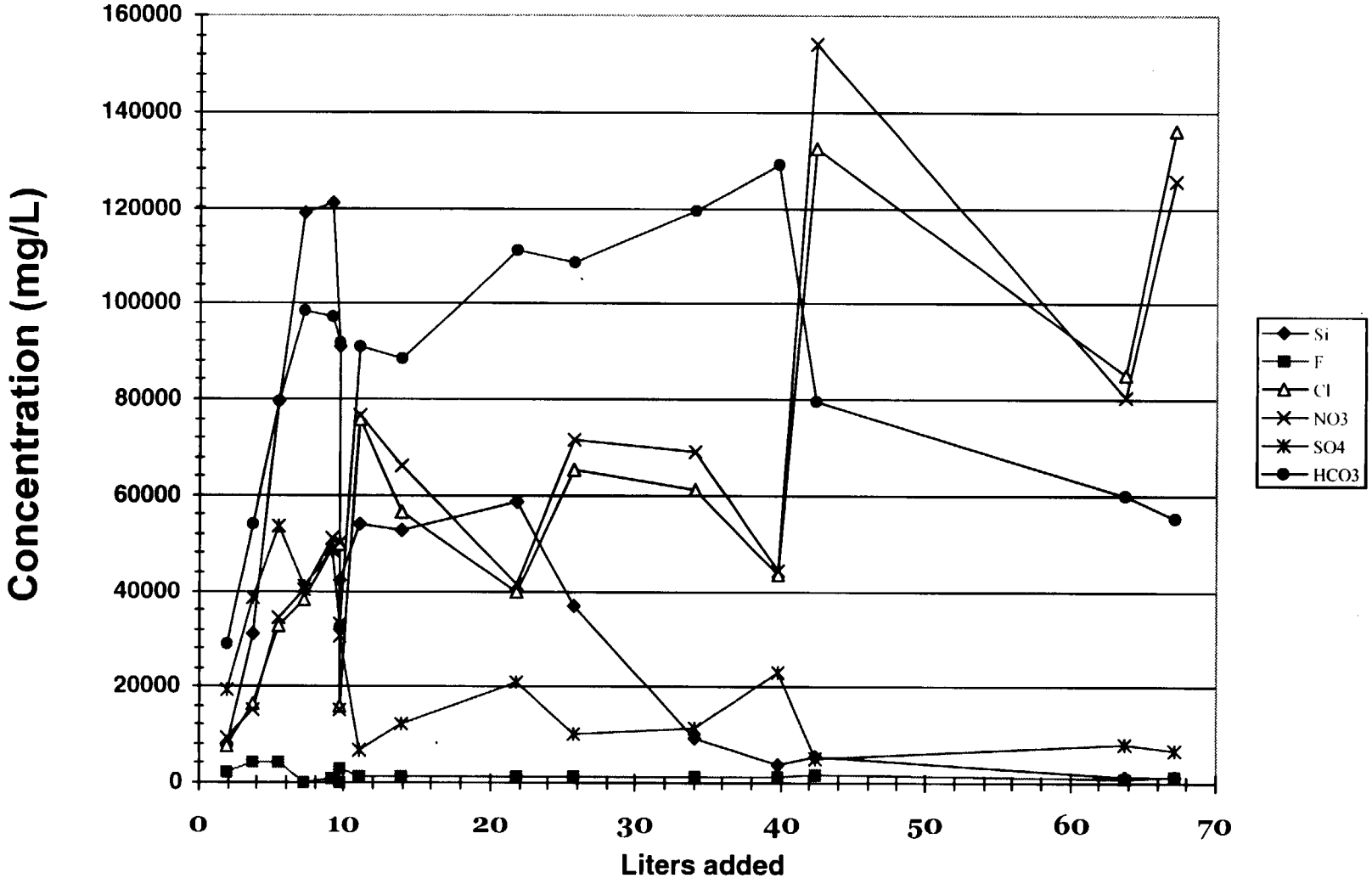
- **Basis for Resolution (Continued)**
  - DOE analysis of Yucca Mountain waters and laboratory test waters includes
    - Anion and cation analysis, including total inorganic carbon
    - pH
    - Boiling points of solutions that have undergone evaporative concentration
    - Mineral/salt precipitate analysis

Range of Water Chemistry Drift Scale Test Ambient Waters

	Concentration (mg/L)	
Ions	ESF-HD PERM-2	ESF-HD PERM-3
Na	61	62
K	7	9
Mg	16.6	17.4
Ca	106	97
Si	31	35
HCO_3	Not obtained	Not obtained
SO_4	111	120
Cl	110	123
NO_3	3	10
F	0.96	0.76

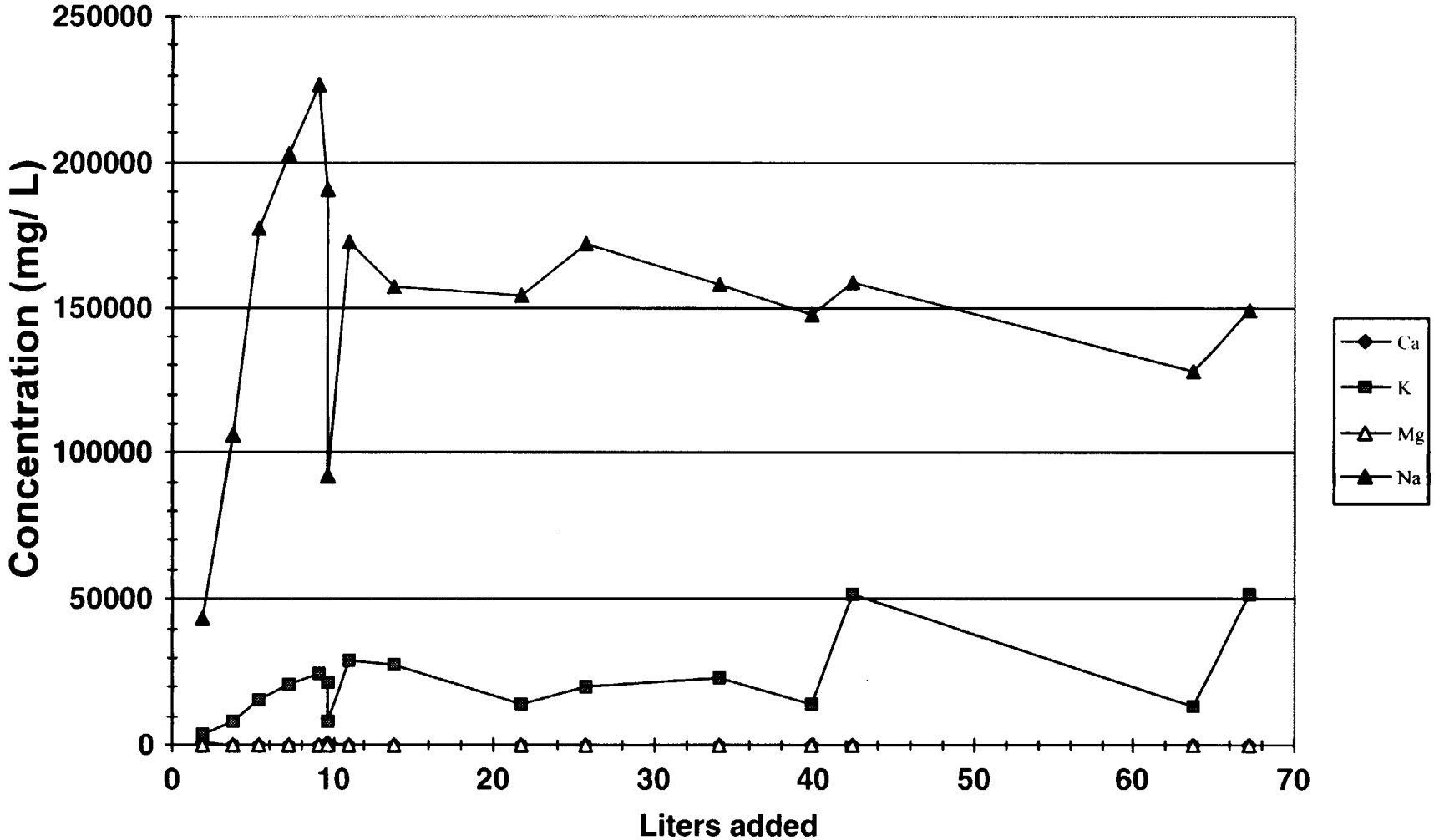
Reference: Drift-Scale Coupled Processes (DST and THC Seepage) Models. MDL-NBS-HS-000001 Rev 01 (work in progress)
Note: Waters were sampled by centrifugal extraction from drill core

Range of Water Chemistry
Anion Analysis of Evaporative Solutions



Reference: Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier. ANL-EBS-MD-000001 Rev 01 (work in progress)

Range of Water Chemistry
Cation Analysis of Evaporative Solutions



Reference: Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier. ANL-EBS-MD-000001 Rev 01 (work in progress)

Range of Water Chemistry
(Continued)

- **Basis for Resolution (Continued)**
  - DOE has used numerous solutions for long-term corrosion testing and evaporative drip testing
    - Bicarbonate-type waters
    - Chloride-sulfate-type waters
    - Moderately concentrated to highly concentrated
    - pH range: 2.7 to 13
    - Temperature range: 60 to 120°C
- **Reference**
  - Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier (ANL-EBS-MD-000001 Rev 00 and future revisions)

Range of Water Chemistry–Trace Elements

- **Basis for Resolution**
  - Trace element concentrations are currently available for
    - EJ-13 (equilibrated J-13) water
    - EJ-13 water is prepared by maintaining actual J-13 well water in contact with crushed Topopah Spring welded tuff at 90°C for extended periods
      - » EJ-13 water is prepared as a corrosion test solution for waste forms
      - » Actual J-13 well water and EJ-13 solutions have been analyzed for trace elements: Li, B, Na, Mg, Al, Si, K, Ca, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, As, Se, Rb, Sr, Ag, Cd, Cs, Ba, Tl, Pb, U
- **DTN: LL001203423121.009**

Testing for Range of Water Chemistry

- **Basis for Resolution**
  - DOE has performed evaporative concentration testing
    - Bicarbonate-type waters (e.g., well J-13 and perched waters)
    - Chloride-sulfate-type waters (e.g., pore waters)
  - DOE is investigating the behavior of added trace element constituents (lead and arsenic) in evaporative concentration tests
  - Mercury may be included as an added trace element in evaporative concentration tests after the need has been established by evaluating mercury concentration in naturally derived waters
  - The reported results from evaporative concentration tests include solution composition, pH, boiling point (where applicable), and mineral precipitates formed

Testing for Range of Water Chemistry
(Continued)

- **Basis for Resolution (Continued)**
  - DOE plans to perform
    - Fractionation studies starting from dilute solutions
    - Trace element analysis on cataloged solutions and solutions in ongoing tests
- **Reference**
  - Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier (ANL-EBS-MD-000001 Rev 00 and future revisions)

Performance of the Titanium Drip Shield

- **Basis for Resolution**
  - Titanium Grade 7 (Ti-0.2Pd) and other grades of titanium are in the corrosion test program
    - Corrosion test program was discussed in Container Life and Source Term Key Technical Issue Technical Exchange
  - Due to the known sensitivity of Ti alloys to solutions containing fluoride, water chemistry testing will determine the extent to which fluoride can concentrate in brines that will form on the drip shield and waste package
    - Testing will incorporate elevated levels of fluoride in dilute waters

Performance of the Titanium Drip Shield
(Continued)

- **References**
  - *General Corrosion and Localized Corrosion of the Drip Shield (ANL-EBS-MD-000004 Rev 00)
  - *Stress Corrosion Cracking of the Drip Shield, the Waste Package Outer Barrier and the Stainless Steel Structural Material (ANL-EBS-MD-000005 Rev 00 ICN 01)
  - *Hydrogen Induced Cracking of Drip Shield (ANL-EBS-MD-000006 Rev 00 ICN 01)
  - *Waste Package Degradation Process Model Report (TDR-WIS-MD-000002 Rev 00 ICN 01)

*Additional information to be provided in future revisions

Conclusions

- Information on the characteristics of water chemistry has been and is being collected to support development of water chemistry models for use in modeling the waste package chemical environment and for corrosion testing of candidate materials for the drip shield and waste package outer barrier
- An appropriate range of water chemistry is incorporated in water chemistry models that are used in modeling the waste package chemical environment and for corrosion testing of the drip shield and the waste package outer barrier

Conclusions
(Continued)

- The performance of the titanium drip shield is part of the corrosion test program which considers the implications of the fluoride concentration
- The corrosion test program considers effects of fluoride concentration on drip shield performance
- DOE considers that the NRC comments about the range of water chemistry and trace elements in the waste package chemical environment related to Subissue 2 have been addressed. The information presented and planned confirmatory studies to examine laboratory solutions that have interacted with introduced materials and effects of elevated levels of fluoride in dilute waters support a status of Closed-Pending for Subissue 2

Backup Slides

Compositions for Selected Corrosion Test Solutions

	Concentration (mg/L)			
Ion	Simulated Dilute Water	Simulated Concentrated Water	Simulated Acidified Water	Simulated Saturated Water
	60 & 90°C	60 & 90°C	60 & 90°C	100*C
K	34	3400	3400	141600
Na	409	40900	40900	48700
Mg	1	<1	1000	0
Ca	0.5	<1	1000	0
F	14	1400	0	0
Cl	67	6700	24250	128000
NO_3	64	6400	23000	1313000
SO_4	167	16700	38600	0
HCO_3	947	70000	0	0
Si	27 (60°C); 49 (90°C)	27 (60°C); 49 (90°C)	27 (60°C); 49 (90°C)	---

Note: Target compositions for solution preparation
Reference: Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier. ANL-EBS-MD-000001 Rev 00

Elemental Concentrations (µg/L)

	J-13 Well Water	EJ-13 Reacted Waters		
Element	J13 5/23/89	EJ13 7/8/98	EJ13 1/18/99	EJ13 4/17/98
Li	47.1	44.6	42.6	47.6
B	94.9	139	131	124
Na	44100	47500	40300	42100
Mg	1660	63	231	198
Al	4.17	664	531	673
Si	28700	42000	32900	32800
K	6590	7950	8650	9400
Ca	14000	7230	3380	8280
V	6.43	7.33	7.75	8.04
Cr	0.739	0.811	0.422	0.787
Mn	<0.59	0.717	6.6	1.14
Fe	<5.97	<5.97	<5.97	<5.97
Co	<0.06	<0.06	<0.06	<0.06
Ni	<2.35	<2.35	<2.35	<2.35
Cu	6.1	<2.17	<2.17	<2.17
Zn	19.3	7.66	19.1	7.76
Ga	<0.05	1.08	1.29	1.46
As	12.6	12.6	14.3	15.8
Se	<39.7	<39.7	<39.7	<39.7
Rb	10.3	19.6	18.7	24.5
Sr	39.7	27.2	17.2	43.3
Ag	<0.09	<0.09	<0.09	<0.09
Cd	<0.89	<0.89	<0.89	<0.89
Cs	1.77	1.58	0.945	1.56
Ba	1.26	0.439	0.408	1.12
Tl	<0.03	0.053	0.043	0.08
Pb	6.08	0.496	0.286	0.586
U	0.701	0.835	<0.03	0.969

DTN: LL001203423121.009

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

Subissue 2: NRC Comments on Data Uncertainties and Sensitivity Studies

Presented to:
DOE-NRC Technical Exchange on Key Technical Issue and Subissues Related to the Evolution of the Near-Field Environment

Presented by:
Ernest Hardin
Civilian Radioactive Waste Management System Management and Operating Contractor

January 9-12, 2001
Pleasanton, CA

YUCCA MOUNTAIN PROJECT

Outline

- **Presentation Objectives**
- **Current Subissue Status**
- **For NRC comments on data uncertainties and sensitivity studies, related to Subissue 4 of the Evolution of the Near-Field Environment Key Technical Issue, this presentation will**
  - Summarize technical basis for comment resolution
  - Give technical basis for current approaches to modeling the in-drift geochemical environment
  - Describe planned actions that will increase confidence in the models
- **Conclusions**

Presentation Objectives

- **Describe the basis for resolving NRC comments on data uncertainties and sensitivity studies associated with Subissue 2 of the Evolution of the Near-Field Environment Key Technical Issue**
- **The DOE has determined that the Precipitates/Salts (PT4) Model for Engineered Barrier System water composition**
  - Produces reasonable agreement with published (ambient temperature) calculations and with available laboratory data from evaporation tests
  - Yields results for different waters representing the range of waters that could be present in the Engineered Barrier System that are similar to experimental data
- **Reference**
  - In-Drift Precipitates/Salts Analysis (ANL-EBS-MD-000045 Rev 00 ICN 02)

Presentation Objectives
(Continued)

- **Limitations exist for models that predict water composition in the Engineered Barrier System**
  - Limitations are being evaluated and addressed by model improvement
  - The approach to understanding thermal-hydrological-chemical coupled processes is based jointly on analysis and laboratory testing
- **Limitations associated with validating models for the Engineered Barrier System physical and chemical environment have been identified and are being addressed through**
  - Model improvements
  - More extensive use of natural and man-made analogs
  - Corrosion process testing

Presentation Objectives
(Continued)

- Existing revisions to the Engineered Barrier System Analysis/Model Report offer enhanced approaches to data uncertainty, alternative models, sensitivity studies, model limitations, and model validation

- Data and modeling issues will continue to be addressed in Analysis/Model Reports and Process Model Report revisions

Current Subissue Status

- Evolution of the Near-Field Environment Issue Resolution Status Report, Rev 03, indicates that Subissue 2 is OPEN

Data Uncertainties

- **NRC Comments**
  - Data uncertainties should be evaluated more rigorously in all DOE Physical and Chemical Environment model Analysis/Model Reports. Inevitable uncertainties in thermodynamic databases, infiltrating water compositions and percolation fluxes, and reactivities, for example, should be evaluated more rigorously to place bounds on parameter values that are output from the models and to constrain their consequences on performance
  - The use of alternate thermodynamic data or slight variations in input parameters, for example, does not capture the full intent of the alternative model criterion
  - Additional sensitivity studies should be performed to identify the limitations of models used to predict coupled THC processes, and the evolution of water and gas compositions with time

Data Uncertainties
(Continued)

- **NRC Comments**
  - Models, data or experiments used to validate Physical and Chemical Environment Models are also subject to critical evaluation. Additional work is needed to evaluate the limitations associated with the validating models, data and experiments, and to provide stronger technical basis for the appropriateness of the comparisons. Discussion with the originators of supporting models, data, and experiments may be needed

Data Uncertainties

- **Basis for resolution**
  - Principal data uncertainties for in-drift models:
    - Laboratory tests may not produce equilibrium conditions
      - » Approach: Equilibrium conditions are discussed in model comparisons with test data
    - Estimated Pitzer coefficients are based on corresponding-states analogy
      - » Approach: Efficacy is addressed through validation arguments using model output and by comparison with published data and models
    - Host-rock water chemistry is represented by a range of compositions
      - » Approach: A plausible boundary condition is used in thermal-hydrological-chemical models; ongoing work will evaluate alternatives
    - Introduced material degradation processes are uncertain
      - » Approach: Steel and cement grout are represented by conservative application of best-available data
  - These uncertainties are addressed in current models through conservative evaluations and multiple data sets

Data Uncertainties
(Continued)

- **References**
  - Thermal Effects on Flow (TEF) – Uncertainties in TSPA-SR (TEF presentation by K. Coppersmith)
  - Engineered Barrier System Degradation, Flow, and Transport Process Model Report (TDR-EBS-MD-000006 Rev 01 work in progress)
  - *Engineered Barrier System: Physical and Chemical Environment Model (ANL-EBS-MD-000033 Rev 01)
  - *Water Distribution and Removal Model (ANL-EBS-MD-000032 Rev 01)
  - *Multi-Scale Thermohydrologic Model (ANL-EBS-MD-000049 Rev 00 ICN 01)
  - In-Drift Precipitates/Salts Analysis (ANL-EBS-MD-000045 Rev 00 ICN 02)
  - Drift-Scale Coupled Processes (DST and THC Seepage) Models (MDL-MBS-HS-000001 Rev 01 is in review)

* Additional information to be provided in future revisions

Sensitivity Studies

- **Basis for resolution**
  - J-13 and matrix pore water compositions are also used for influent water (compared to results obtained with the abstracted thermal-hydrological-mechanical model output compositions)
  - Steel corrosion rates are determined/evaluated with different water compositions (estimate possible range of corrosion rates)
  - Effects of drift seepage on the in-drift thermodynamic environment have been evaluated and found to be minor
  - Mixing and dispersion of gas-phase constituents produced/consumed in the drifts associated with thermal-hydrologic circulation in the host rock is being evaluated

Sensitivity Studies
(Continued)

- **References**
  - In-Drift Precipitates/Salts Analysis (ANL-EBS-MD-000045 Rev 00 ICN 02)
  - *Engineered Barrier System: Physical and Chemical Environment Model (ANL-EBS-MD-000033 Rev 01)
  - Water Distribution and Removal Model (ANL-EBS-MD-000032 Rev 01)
  - Engineered Barrier System Process Model Report Rev 01 is work in progress

*Additional information to be provided in future revisions

Model Validation and Technical Basis

- **Basis for Resolution**
  - DOE is focusing on data and model issues with greatest potential to affect repository performance
    - Drip shield/waste package chemical environment is being addressed by testing performed for resolution of the Container Life and Source Term Key Technical Issue
    - DOE is considering developing additional laboratory test data to constrain the interpolative Low Relative Humidity Salts Model
    - The Pitzer (PT4) database and certain EQ3/6 numerical features are being revised to improve confidence over a broader range of environmental conditions
    - Additional sensitivity testing will be performed for planned Analysis/Model Report revisions
  - DOE will continue to address data uncertainty and sensitivity testing in revisions to Analysis/Model Reports and Process Model Reports

Model Validation and Technical Basis
(Continued)

- **References**
  - In-Drift Precipitates/Salts Analysis (ANL-EBS-MD-000045 Rev 00 ICN 02)
  - Engineered Barrier System: Physical and Chemical Environment Model (ANL-EBS-MD-000033 Rev 01)
  - Engineered Barrier System Degradation, Flow, and Transport Process Model Report (TDR-EBS-MD-000006 Rev 01 work in progress)
  - *Waste Package Degradation Process Model Report (TDR-WIS-MD-000002 Rev 00 ICN 01)

*Additional information to be provided in future revisions

Conclusions

- Data uncertainty and sensitivity testing are included in existing analysis model reports, particularly to address uncertainty in the boundary condition on the drift environment and the implementation of the Pitzer approach for modeling water compositions
- DOE will continue to address data uncertainty and sensitivity testing in revisions to analysis/model reports and process model reports

Conclusions (Continued)

- DOE considers the NRC comments about data uncertainties and sensitivity studies related to Subissue 2 have been addressed. The information presented, planned sensitivity studies to identify limitations of models used to predict coupled thermal-hydrological-chemical processes and evolution of water and gas, and studies being considered to update the EQ3/6 code support a status of Closed-Pending for Subissue 2
- DOE considers this presentation, in conjunction with preceding ones, provides sufficient information to status Subissue 2 as Closed-Pending

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

Addendum to Data Uncertainties and Sensitivity Studies Presentation for Subissue 2: Validation Approach for the Precipitates/ Salts Model

Presented to:
DOE-NRC Technical Exchange on the Evolution of the Near-Field Environment Key Technical Issue

Presented by:
Ernest Hardin
Civilian Radioactive Waste Management System Management and Operating Contractor

January 9-11, 2001
Pleasanton, California

YUCCA MOUNTAIN PROJECT

Precipitates/Salts Model

Comparison of Precipitates/Salts Model (PT4) Results for a Canadian Shield Brine at Ambient Temperature, vs. Published Results Using the Modeling Approach of Harvie, Moeller, and Weare (1984)

Input Parameter	Units	Value	
pH	None	5.0	
Na^+	mg/L	45,000	
K^+	mg/L	199	
Ca^{2+}	mg/L	64,000	
Mg^{2+}	mg/L	5100	
Cl-	mg/L	207,000	
SO_4^{2-}	mg/L	284	
HCO_3^-	molal	0.032428	
Output Parameter	**Units**	**PT4**	**HMW**
Activity of water	None	0.7209	0.7202
Ionic strength	molal	8.550	8.551
SI, calcite ($CaCO_3$)	None	+1.588	+1.918
SI, dolomite [$CaMg(CO_3)_2$]	None	+3.612	+3.451
SI, gypsum ($CaSO_4.2H_2O$)	None	+0.174	+0.333
SI, anhydrite ($CaSO_4$)	None	+0.213	+0.400
SI, halite (NaCl)	None	-0.158	-0.136
SI, sylvite (KCl)	None	-2.472	-2.481

Excerpted from the Engineered Barrier System Physical and Chemical Environment Model ANL-EBS-MD-000033 Rev. 01, Tables 6.7-1 and 6.7-2.

Precipitates/Salts Model

Comparison of Precipitates/Salts Model (PT4) Results for a Dead Sea Brine at Ambient Temperature, vs. Published Results Using the Modeling Approach of Harvie, Moeller, and Weare (1984)

Input Parameter	Units	Value	
pH	None	(calculated)	
Na^+	molal	1.7519	
K^+	molal	0.1739	
Ca^{2+}	molal	0.4274	
Mg^{2+}	molal	1.5552	
Cl-	molal	5.8098	
SO_4^{2-}	molal	0.0063	
HCO_3^-	molal	0.00392	
$\log_{10} P_{CO2}$	None	-3.5	
$\log_{10} P_{O2}$	None	-0.7	
Output Parameter	**Units**	**PT4**	**HMW**
Activity of water	None	0.7538	0.7502
pH	None	7.42	7.43
Ionic strength, molal	molal	7.841	7.840
SI, calcite ($CaCO_3$)	None	2.075	2.013
SI, dolomite [$CaMg(CO_3)_2$]	None	6.095	5.123
SI, gypsum ($CaSO_4.2H_2O$)	None	-0.083	-0.002
SI, anhydrite ($CaSO_4$)	None	-0.014	0.030
SI, halite (NaCl)	None	-0.434	-0.352
SI, sylvite (KCl)	None	-1.086	-1.065

Excerpted from the Engineered Barrier System Physical and Chemical Environment Model ANL-EBS-MD-000033 Rev. 01, Tables 6.7-5 and 6.7-6.

Precipitates/Salts Model

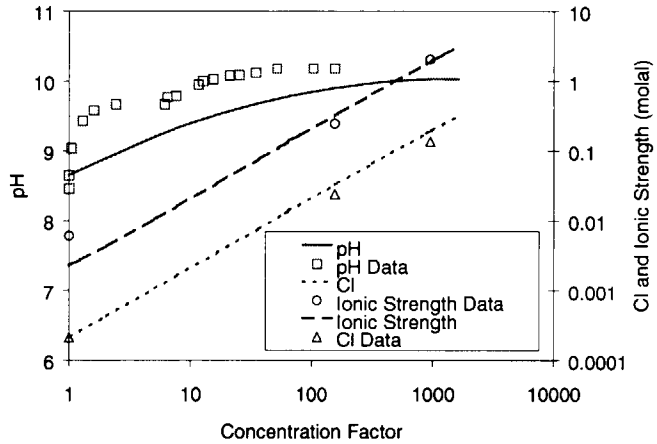
Comparison of Handbook Aqueous Solubilities for Sodium and Potassium Salts at 100°C With Calculated Values

Soluble Salt	Handbook Aqueous Solubility at 100°C (molal)	Predicted Pure-Phase Solubility at 100°C [A] (molal)	% Error [(Predicted Value ÷ Handbook Value) x 100 − 100]
NaCl	6.70	7.21	+7.6
KCl	7.60	6.12	-19.5
$Na_2CO_3 \cdot H_2O$	4.2 or 3.67 [B]	3.99	-5.0 or +8.7
K_2CO_3	11.3	> 10 [C]	Note C
NaF	1.21	1.01	-16.5
KF	26 (at 80°C)	> 10 [C]	Note C
Na_2SO_4	3.01	1.55	-48.5
K_2SO_4	1.38	0.83	-39.9
$NaNO_3$	21.2	3.60	-82.9
KNO_3	24.4	3.60	-85.2

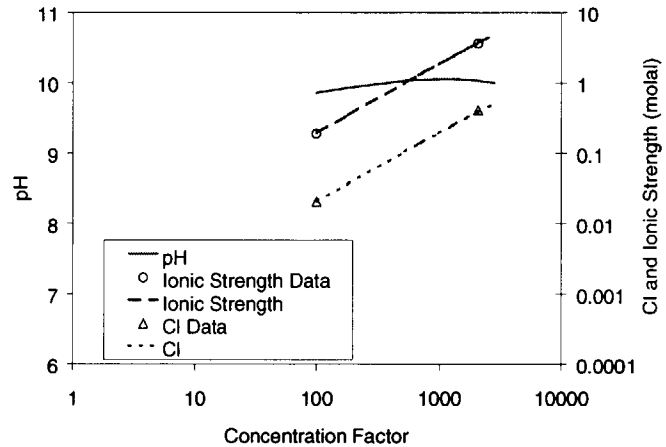
[A] High-Relative-Humidity Salts Model (PT4 Pitzer database) [B] Values from alternative sources
[C] Beyond range of EQ3/6 V7.2b implementation

Precipitates/Salts Model, Continued

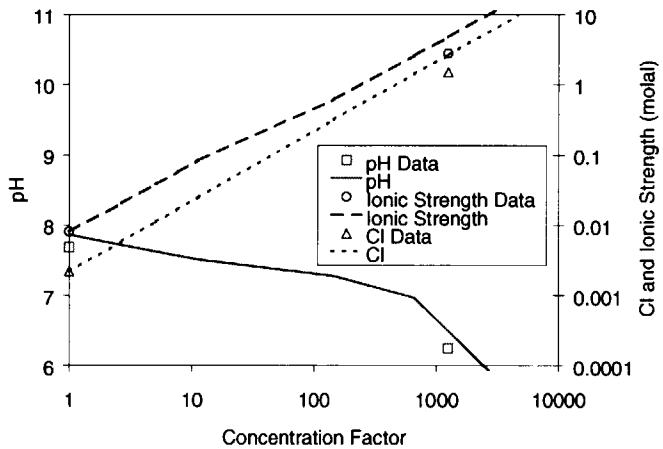
A



B



C



Precipitates/Salts Model Predictions vs. Laboratory Test Data

A) J-13 evaporation at 85°C
B) 100x average J-13 evaporation at 90°C and 85% relative humidity
C) Topopah Spring Tuff pore water evaporation at 75°C

Comparison of Results from Evaporation Tests to Precipitates/Salts Model Predictions

Component (Concentrations are molal except pH)	Evaporation of Synthetic Average J-13 Well Water at 85°C (Concentration factor: 157)		Evaporation of Synthetic 100x Average J-13 Well Water at 90°C and 85% Relative Humidity (Effective concentration factor: 2,070)		Evaporation of Synthetic Topopah Spring Tuff Pore Water at 75°C (Concentration factor: 1,243)	
	Experimental Results	Model Predictions	Experimental Results	Model Predictions	Experimental Results	Model Predictions
pH	10.18	9.90	not reported	10.03	6.25	6.50
Ionic strength	2.45E-01	4.43E-01	3.60E+00	3.69E+00	2.79E+00	4.81E+00
Na	2.30E-01	3.07E-01	3.32E+00	3.44E+00	2.59E-01	4.33E-01
K	1.43E-02	1.95E-02	2.77E-01	2.48E-01	7.11E-02	1.30E-01
Ca	2.99E-05	1.42E-06	8.98E-04	1.75E-06	3.90E-01	5.50E-01
Mg	2.06E-06	1.84E-08	0.00E-00 [A]	2.16E-06	2.25E-01	5.12E-01
Cl	2.39E-02	3.29E-02	4.07E-01	3.87E-01	1.50E+00	2.67E+00
CO_3	7.04E-02	1.11E-01	8.95E-01	1.15E+00	< 5.74E-04 [B]	4.56E-05
SO_4	2.25E-02	3.08E-02	3.10E-01	3.19E-01	2.16E-02	6.14E-03
SiO_2	1.66E-02	2.82E-03	not included in test		8.54E-03	4.82E-04
F	1.30E-02	1.97E-02	1.91E-01	1.97E-01	< 3.04E-02 [B]	1.53E-03
NO_3	1.69E-02	2.01E-02	2.27E-01	2.22E-01	not measured	2.15E-01

NOTES:

A. Zero concentration reported; no detection limit available

B. Below detection limit

Reference: In-Drift Precipates/Salts Analysis ANL-EBS-MD-000045, Rev 00, ICN 02

Precipitates/Salts Model Conclusions

- **Comparison with published data and models at near-ambient temperature:**
  - Dead Sea brine, Canadian Shield brine, and other examples show agreement with the Harvie,Moeller, & Weare (HMW) approach
- **Comparison with lab test data at elevated-temperature:**
  - Experimental pH data are predicted within a pH unit or better
  - Chloride and ionic strength are predicted within a factor of 2
  - Handbook solubilities for ten simple salts (solubilities > 1 molal) are predicted within an order of magnitude and often within a factor of 2 or better
- **Uncertainties in use of elevated temperature data:**
  - Mineral equilibrium (possibly chalcedony, calcite, sepiolite)
  - CO_2 fugacity over evaporating solutions

Precipitates/Salts Model Conclusions, Continued

- DOE considers the Precipitates/Salts Model is valid for its intended use as a component of the current Total System Performance Assessment (subject to the accuracy constraints indicated above)
- DOE considers the NRC comments concerning the use of laboratory test data for model validation have been addressed, and that this presentation in conjunction with preceding ones provides sufficient information to status Subissue 2 as Closed-Pending

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

Subissue 3: NRC Comments on Thermal-Hydrological-Chemical Effects on Radionuclide Release

Presented to:
DOE-NRC Technical Exchange on Key Technical Issue and Subissues Related to Evolution of the Near-Field Environment

Presented by:
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YUCCA MOUNTAIN PROJECT

Outline

- **Presentation Objectives**
- **Current Subissue Status**
- **For NRC comments on thermal-hydrological-chemical effects on radionuclide release, related to Subissue 3 of the Evolution of the Near Field Environment Key Technical Issue, this presentation will**
  - Summarize technical basis for resolution of NRC comments
  - Identify basis documents (References)
  - Describe future actions that will provide basis for final closure of Subissue 3
- **Conclusions**

Presentation Objectives

- **Describe the basis for resolving NRC comments related to thermal-hydrological-chemical effects on radionuclide release**
- **Department of Energy has determined that**
  - Limitations exist for the In-Package Chemistry Model, but they are being evaluated and addressed by model and data improvement
  - The approach to understanding thermal-hydrological-chemical effects on radionuclide release is based on integrated testing and analyses

Thermal-Hydrological-Chemical Effects on Radionuclide Release

- **NRC Comments**
  - Abstraction of in-package chemistry ignores the potential effect of early-state high temperature phenomena. The chloride concentration used in the abstraction is equal to that of J-13 well water. This value ignores the potential increase in chloride concentration due to evaporation of water prior to its entry into the waste packages
- **Basis for Resolution**
  - High-temperature phenomena need not be considered because waste package failure does not occur until after 10,000 years (WAPDEG Analysis of Waste Package and Drip Shield Degradation Analysis/Model Report ANL-EBS-PA-000001 Rev 00 ICN 01)

Thermal-Hydrological-Chemical Effects on Radionuclide Release (Continued)

- **Basis for Resolution (Continued)**
  - Preliminary information indicates evaporative concentration effects on seepage composition prior to entering the waste package will not be significant during the post 10,000 year period when waste package failure occurs (Near-Field Environment Process Model Report TDR-NBS-MD-000001 Rev 00 ICN03)
  - Verification analyses are planned to support this assumption

Thermal-Hydrological-Chemical Effects on Radionuclide Release (Continued)

- **NRC Comment**
  - The abstraction also ignored the potential increase in fluoride concentration, which could enhance cladding degradation due to evaporation effects
- **Basis for Resolution**
  - The cladding localized corrosion model is conservative and assumes all fluoride that enters the waste package is utilized in zirconium corrosion (Clad Degradation-Summary and Abstraction ANL-WIS-MD-000007 Rev 00)
  - Therefore, evaporative concentration of fluorides inside the waste package will not have any effect on the model

Thermal-Hydrological-Chemical Effects on Radionuclide Release (Continued)

- **Basis for Resolution (Continued)**
  - Preliminary information indicates evaporative concentration of fluoride in the near field prior to seepage entering the waste package will not be significant until the post 10,000 year period when waste packages fail (Near-Field Environment Process Model Report TDR-NBS-MD-000001 Rev 00 ICN 03)
  - Verification analyses are planned to support this assumption

Thermal-Hydrological-Chemical Effects on Radionuclide Release (Continued)

- **NRC Comment**
  - The abstraction of in-package chemistry also ignores the potential interaction with grouted rock bolts, and interactions with other engineered materials on the chemistry of water inside waste packages. A justification used in the analysis model report is that the residence time of water in the waste package will be too short to allow reactions between the water and the waste package materials to occur. This justification is considered inadequate
- **Basis for Resolution**
  - Grout surrounding the rock bolts will be carbonated and neutralized well before waste package failure occurs and therefore will not affect chemistry of seepage entering the waste package (Engineered Barrier System Physical and Chemical Environment Model, ANL-EBS-MD-000033 Rev 00 ICN 01)
  - Other materials, such as the ground support system, will have a negligible impact on seepage chemistry (In-Drift Corrosion Products ANL-EBS-MD-000041 Rev 00), especially at waste package failure times

Thermal-Hydrological-Chemical Effects on Radionuclide Release (Continued)

- **NRC Comment**
  - The abstraction of commercial spent nuclear fuel (CNSF) degradation ignored the potential effects of several processes. The possible effect of radiolytic production of acid from moist air on the dissolution of uranium fuel is not adequately addressed. The effect of periodic wet and dry conditions on the dissolution rate is not considered
- **Basis for Resolution**
  - The CSNF Waste Form Degradation Analysis/Model Report (ANL-EBS-MD-000015 Rev 00) addresses radiolysis
  - pH suppression is addressed in the In-Package Chemistry Analysis/Model Report (ANL-EBS-MD-000050 Rev 01)
  - The CSNF Waste Form Degradation Analysis/Model Report (ANL-EBS-MD-000015 Rev 00) uses rate laws for constantly saturated conditions, which is more conservative than the wetting/drying scenario

Thermal-Hydrological-Chemical Effects on Radionuclide Release (Continued)

- **NRC Comment**
  - The Analysis Model Report on in-package chemistry abstraction does not provide enough information on the corrosion rate used in the abstractions. It is not clear if the high rate is related to localized corrosion or the highest rate for uniform corrosion. It is not clear if the corrosion rate used in this Analysis Model Report is consistent with WAPDEG predictions. What references were used for the degradation rates of the waste package components? Are the rates taken from the references relevant to the specific in-package environment being simulated?
- **Basis for Resolution**
  - Improved description and selection of corrosion rates are provided in the revised In-Package Chemistry Analysis/Model Report (ANL-EBS-MD-000050 Rev 01)
  - New corrosion rates are consistent with data obtained from long-term corrosion test facility experiments done under conditions relevant to Yucca Mountain, which is the source for WAPDEG predictions (Waste Package Degradation Process Model Report TDR-WIS-MD-000002 Rev 00 and McCright 1998)

Thermal-Hydrological-Chemical Effects on Radionuclide Release (Continued)

- **NRC Comment**
  - The Analysis Model Report on in-package chemistry summary states that the input surface areas, waste package component dissolution rates, and thermodynamic database have yet to be verified. The DOE needs to provide the status of this verification work
- **Basis for Resolution**
  - The thermodynamic database has been verified (M0009THRMODYN.001)
  - Studies of the sensitivity of chemistry to surface areas and corrosion rates are being considered for the quantification of uncertainty
  - DOE plans to complete sufficient verification work by the submittal of the License Application

Thermal-Hydrological-Chemical Effects on Radionuclide Release (Continued)

- **NRC Comment**
  - There is no attempt in the Analysis Model Report on in-package chemistry abstraction to explain how good a fit the response surfaces are to the values computed using EQ/6
- **Basis for Resolution**
  - The current revision of the In-Package Chemistry Abstraction Analysis/Model Report (ANL-EBS-MD-000037 Rev 01) provides fit information (R-squared values) for the response surfaces. For example, the pH R^2 ranges from about 0.7 to 0.99, which indicates a good fit

Thermal-Hydrological-Chemical Effects on Radionuclide Release (Continued)

- **NRC Comment**
  - It is claimed that waste form degradation can be adequately modeled with a 25°C thermodynamic database. It is claimed that many of the thermodynamic parameters are not strongly sensitive to temperature over the range 25 to 100°C, hence the broad scale features of the calculated fluid compositions are considered independent of temperature. However, no evidence of the insensitivity of calculated results was provided. The DOE needs to conduct sensitivity analyses to determine if temperature effects is important

Thermal-Hydrological-Chemical Effects on Radionuclide Release (Continued)

- **Basis for Resolution**
  - The basis for using 25°C thermodynamic date to model processes that might occur at somewhat higher temperatures is that many of the input thermodynamic parameters are not strongly sensitive to temperature over the range of 25 to 100°C (see the temperature-dependent equilibrium constants in datao.pvb). Hence, the broad scale features of the output fluid compositions are deemed independent of temperature (In-Package Chemistry Analysis/Model Report (ANL-EBS-MD-000050 Rev 01)

Thermal-Hydrological-Chemical Effects on Radionuclide Release (Continued)

- **NRC Comment**
  - No technical basis is provided for ignoring the potential temperature dependence of degradation rates of waste package components in the analyses
- **Basis for Resolution**
  - Because waste packages fail after temperatures have cooled to less than 100°C, high temperature waste package component degradation processes are not expected to occur (WAPDEG Analysis of Waste Package and Drip Shield Degradation Analysis Model Report ANL-EBS-PA-000001)
  - Moreover, degradation rates of waste package components are conservative, because they are held fixed at their high rates for the entire calculation period. Degradation rates will tend to decrease with decreasing temperature (In-Package Chemistry Analysis/Model Report ANL-EBS-MD-000050 Rev 01)
  - Therefore, the current approach is conservative

Thermal-Hydrological-Chemical Effects on Radionuclide Release (Continued)

- **NRC Comment**
  - In the Analysis Model Report on in-package chemistry abstraction, the abstraction of ionic strength for times greater than 1,000 years, the average value of ionic strengths calculated from the process level modeling was used. The DOE needs to provide a better technical justification for not using the more conservative approach of minimum ionic strength
- **Basis for Resolution**
  - DOE does not use the minimum ionic strength approach because the revised abstraction of the In-Package Chemistry Abstraction Analysis/Model Report (ANL-EBS-MD-000050 Rev 01) has improved the resolution and treatment of ionic strength calculations by considering an additional time period and defining ionic strength distributions for each time period that will be sampled in Total System Performance Assessment calculations

Thermal-Hydrological-Chemical Effects on Radionuclide Release (Continued)

- **NRC Comments**
  - The evolution of the in-package chemistry depends on the rate of dissolution of waste package components assumed in the calculations. The dissolution rates of stainless steels assumed for the analysis are particularly important because degradation of stainless steels lead to lower pH. If the dissolution rate assumed in the calculation is improperly low, the effect of low pH on calculated dose may not be observed from the results. The dissolution rate assumed for Type 316 stainless steel and borated stainless steel is one order of magnitude lower than the rate measured experimentally for Alloy 22, which is counter-intuitive to the known higher corrosion resistance of Alloy 22 compared to stainless steels. The DOE needs to provide technical bases for the corrosion rates used in their calculations

Thermal-Hydrological-Chemical Effects on Radionuclide Release (Continued)

- **Basis for Resolution**
  - Improved description and selection of corrosion rates have been provided in the revised In-Package Chemistry Analysis/Model Report (ANL-EBS-MD-000050)
  - New corrosion rates are consistent with data obtained from long-term corrosion test facility experiments done under conditions relevant to the Yucca Mountain Project
  - High rates were chosen to remain conservative
  - The basis for the NRC statement that corrosion rates for Type 316 stainless steel and borated stainless steel are an order of magnitude lower than the experimentally measured rate for Alloy 22 is not clear
    - The median corrosion rate for Alloy 22 is about 4.5×10^{-5} mm/yr (CAL-EBS-PA-000002 Rev 01)
    - The median corrosion rate for stainless steel is about 2×10^{-3} mm/yr (ANL-EBS-PA-000005 Rev 00)

Thermal-Hydrological-Chemical Effects on Radionuclide Release (Continued)

- **NRC Comments**
  - The analysis assumes water may circulate freely enough in the partially degraded waste package so that all degraded solid products may react with each other through the fluid. Also, an assumption is made that circulation and mixing of water occurs inside the package that allows complete exposure of waste package components to incoming fluids. The analyses lumped all components into a single mass for purposes of calculating the chemistry of water that interacts with waste package components. It was claimed that this assumption maximizes the amount of waste package degradation. However, the assumption ignores the development of local environments that are more corrosive than calculated based on a volume-averaged basis

Thermal-Hydrological-Chemical Effects on Radionuclide Release (Continued)

- **Basis for Resolution**
  - Analyses thus far focused on well-understood, bulk-scale chemical processes that are likely to dominate the in-package chemical environment
  - Local environments may be present but they are unlikely to have a significant effect on overall waste form dissolution and radionuclide release (In-Package Chemistry Analysis/Model Report ANL-EBS-MD-000050)
  - Future analyses are planned to verify this assumption

Thermal-Hydrological-Chemical Effects on Radionuclide Release (Continued)

- **NRC Comments**
  - It is stated in the Analysis/Model Report on in-waste package chemistry that it is not possible to fully validate the model at this time or to assign absolute confidence limits to in-package chemistry outputs. The DOE should identify confirmatory steps that will be conducted to validate the models
- **Basis for Resolution**
  - Model validation is more fully discussed in the In-Package Chemistry Analysis/Model Report (ANL-EBS-MD-000050 Rev 01)
  - Additional analysis will be required before experimental validation is started. Examples of analysis that could be done include modeling of Argonne Drip Tests and verifying acid production from corrosion of stainless steels

Thermal-Hydrological-Chemical Effects on Radionuclide Release (Continued)

- **NRC Comments**
  - DOE predictions of in-package chemistry based on the EQ3/6 code have not been verified by empirical observations. In particular, staff has concerns regarding the use of the EQ3/6 code because it does not incorporate electrochemical reactions. Experiments to simulate certain aspects of waste package geometry and materials may aid in gaining confidence in the EQ3/6 results
- **Basis for Resolution**
  - Model validation is more fully discussed in the In-Package Chemistry Analysis/Model Report (ANL-EBS-MD-000050 Rev 01)
  - Additional analysis are needed before experimental validation is started. Examples of analysis that could be done include modeling of Argonne Drip Tests and verifying acid production from corrosion of stainless steels

References

- Abstraction of Models for Stainlesss Steel Structural Material Degradation (ANL-EBS-PA-000005 Rev 00)
- Calculation of General Corrosion Rate of Drip Shield and Waste Package Outer Barrier to Support WAPDEG Analysis (CAL-EBS-PA-000002 Rev 01)
- Clad Degradation-Summary and Abstraction (ANL-WIS-MD-000007 Rev 00)
- CSNF Waste Form Degradation (ANL-EBS-MD-000015 Rev 00)
- Engineered Barrier System Physical and Chemical Environment Model (ANL-EBS-MD-000033 Rev 00 ICN 01)
- In Drift Corrosion Products (ANL-EBS-MD-000041 Rev 00)
- In-Package Chemistry Abstraction (ANL-EBS-MD-000037 Rev 01)
- In-Package Chemistry Summary (ANL-EBS-MD-000050 Rev 01)
- McCright, R.D. 1998. Corrosion Data and Modeling, Update for Viability Assessment. Volume 3 of Engineered Materials Characterization Report. UCRL-ID-119564 Rev 1.1 ACC:Mol.1998.0806.0177

References
(Continued)

- Near Field Environment Process Model Report (TDR-NBS-MD-000001 Rev 00 ICN 03)
- WAPDEG Analysis of Waste Package and Drip Shield Degradation Analysis/Model Report (ANL-EBS-PA-000001 Rev 00 ICN 01)
- Waste Package Degradation Process Model Report (TDR-WIS-MD-000002 Rev 00)

Conclusions

- New supporting analyses and information are included in revisions of the In-Package Chemistry Process and Abstraction Model Analysis/Model Reports
- Additional analyses and testing have been planned to verify existing information and improve the basis for model validation
- DOE considers that the NRC comments about thermal-hydrological-chemical effects on radionuclide release related to Subissue 3 have been addressed. The information presented and additional studies that are planned and being considered to confirm expectations regarding thermal-hydrological-chemical effects on radionuclide release support a status of Closed-Pending for Subissue 3