

REVIEW BY THE NUCLEAR REGULATORY COMMISSION  
OFFICE OF NUCLEAR MATERIAL SAFETY AND SAFEGUARDS  
OF THE DEPARTMENT OF ENERGY AGREEMENT RESPONSES RELATED TO THE  
PROPOSED GEOLOGIC REPOSITORY AT YUCCA MOUNTAIN, NEVADA:  
IN-DRIFT CHEMICAL ENVIRONMENT-RELATED AGREEMENTS FOR KEY TECHNICAL  
ISSUES "EVOLUTION OF THE NEAR-FIELD ENVIRONMENT" (ENFE 2.09, 2.11, 2.15),  
"TOTAL SYSTEM PERFORMANCE ASSESSMENT AND INTEGRATION" (TSPAI 3.13), AND  
"GENERAL" (GEN 1.01, COMMENTS 50, 93, 98, 110, 113, AND 118)

## 1.0 INTRODUCTION

The U.S. Nuclear Regulatory Commission's (NRC) issue resolution goal during this interim preclicensing period is to assure the U.S. Department of Energy (DOE) has assembled enough information about a given issue for NRC to accept a license application for review. Resolution by NRC during preclicensing does not prevent anyone from raising any issue for NRC consideration during the licensing proceedings. It is equally important to note that resolution of an issue by NRC during the preclicensing period does not prejudice the NRC evaluation of the issue during the licensing review. Issues are resolved by NRC during preclicensing when the staff has no further questions or comments about how DOE is addressing an issue. Pertinent new information could raise new questions or comments about a previously resolved issue.

By a letter dated November 25, 2003, DOE submitted a report titled "Technical Basis Document No. 5: In-Drift Chemical Environment" (Bechtel SAIC Company, LLC, 2003a) to satisfy the informational needs of numerous Key Technical Issue (KTI) agreement items pertaining to the in-drift chemical environment and to respond to issues raised by NRC about the chemical environment on the surfaces of the waste package and drip shield at the potential repository at Yucca Mountain, Nevada. The information was requested by NRC during previous technical exchanges in September 2000, January 2001, August 2001, and September 2001. The specific agreements, which are addressed in the technical basis document, are categorized according to five different KTIs:

- (i) Evolution of the Near-Field Environment (ENFE) agreements 1.05, 2.04, 2.05, 2.06, 2.09, 2.10, 2.11, 2.13, 2.14, 2.15, and 2.17
- (ii) Container Life and Source Term (CLST) agreement 1.01
- (iii) Total System Performance Assessment and Integration (TSPAI) agreements 3.09, 3.12, and 3.13
- (iv) Thermal Effects on Flow (TEF) agreement 2.04
- (v) General (GEN) agreement 1.01, Comments 47, 50, 81, 93, 98, 104, 109, 110, 113, 118, 122, and 124

For all 17 agreements and 12 comments, DOE stated in the technical basis document that it has satisfied the NRC information needs regarding the agreements and that all agreements

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should be considered complete. Section 4.0 of this report provides the NRC evaluation of the extent to which the DOE submittal satisfies the informational requirements of four of the agreements (ENFE 2.09, 2.11, 2.15, and TSPAI 3.13) and six of the GEN 1.01 Comments (50, 93, 98, 110, 113, and 118). NRC evaluation of the extent to which the DOE submittal satisfies the requirements of the other agreements will be provided in a separate document.

## 2.0 CATEGORIES OF THE AGREEMENTS

In Appendices A, B, F, and H of the technical basis document, DOE identified four categories of KTI agreements as being satisfied by the information provided in the report:

- Agreements Pertaining to Credible Range of Brine Water Chemistry and Consistency Between Corrosion Testing Environments and Models [TSPAI 3.13 and GEN 1.01 (Comments 50, 113, and 118)]
- Agreements Pertaining to Uncertainty and Variability in the Near-Field Geochemical Environment (GEN 1.01, Comments 93, 98, and 110)
- Agreement Pertaining to the Modeling of Salt Interactions at Low Relative Humidity (ENFE 2.09 and ENFE 2.15)
- Agreement Pertaining to the Kinetics of Chemical Processes (ENFE 2.11)

The wording of the individual agreements precedes the DOE-provided technical content summarized in Section 3.0.

## 3.0 TECHNICAL INFORMATION PROVIDED IN THE DOE AGREEMENT RESPONSE

3.1 Agreements Pertaining to Credible Range of Brine Water Chemistry and Consistency Between Corrosion Testing Environments and Models [TSPAI 3.13 and GEN 1.01 (Comments 50, 113, and 118)]

### 3.1.1 TSPAI 3.13 Agreement (Reamer, 2001a)

Provide a comparison of the environments for corrosion predicted in the models, to the testing environments used to define empirical corrosion rates in revised documentation (ENG 3.2.1). DOE will provide a comparison of the environments for corrosion predicted in the models, to the testing environments utilized to define empirical corrosion rates in revised documentation consistent with the scope and schedule for existing agreement item CLST 1.1.

Appendix A of the DOE Technical Basis Document (Bechtel SAIC Company, LLC, 2003a) provides information related to agreement TSPAI 3.13. This agreement requests DOE to compare its abstractions of near-field chemical environment to the testing environments used in

its corrosion experiments. In the technical basis document, DOE provides the range of environments projected to form within the repository because of water seepage. These seepage waters were categorized into 11 bins, or water types, based on their chemical

composition and are characterized by their dominant ionic species at relative humidity of 98 percent and during conditions just before dryout. For each bin, an associated brine type (calcium chloride, carbonate, and sulfate) corresponding to the endpoint composition of the bin is identified, as well as the aqueous test solution used in DOE corrosion studies associated with the particular brine type (Table A–1 of the technical basis document). DOE also projected environments forming in a dust–deliquescence scenario, categorized into 6 bins based on their composition at 98-percent relative humidity. A comparison of the end-point chemistry after evaporation and the corrosion test solution is presented in Table A–5 of the technical basis document. An alternative method to predict water chemistries for the dust-deliquescence scenario yielded similar results (Table A–4 of the technical basis document). DOE provided rationale for the environments in the corrosion tests, particularly those in the Long-Term Corrosion Test Facility for defining general corrosion rates for long-term extrapolation.

3.1.2 (Comment 50) (Reamer, 2001b)

- What is the probability of the formation of sufficient conditions leading to localized corrosion?

If none, then

- Which solution compositions hitting the waste package and evaporating could lead to sufficient environmental conditions for the onset of localized corrosion?
- What is the probability that such initial solution compositions could be established?”

(Comment 113) (Reamer, 2001b)

Page 7T-1: Does the pore water composition shown in Table 7.3.1-2 suggest that the waters in the Yucca Mountain system already exhibit evidence of evolving to a Ca-Mg-Cl type system, thereby making the evolution of the waters due to thermal influences more likely to end up in the Ca-Mg-Cl system (the concentration factors of Ca, Mg, and Cl from fracture to pore water are much larger than for NO<sub>3</sub>)?

(Comment 118) (Reamer, 2001b)

DOE’s assessment of deliquescence humidity did not consider the mixed salt effect. Mixed salts may lower the [deliquescence] points below that of pure salts.

(Comments 50, 113, and 118) (Reamer, 2001b)

Appendix A of the DOE Technical Basis Document (Bechtel SAIC Company, LLC, 2003a) provides information about GEN 1.01, Comments 50, 113, and 118. GEN 1.01, comments 50, 113, and 118 are related to NRC concerns about the lack of sufficient information on the (i) probability of environmental conditions necessary for localized corrosion, (ii) formation of calcium-magnesium-chloride-rich water from pore water, and (iii) the effect of mixed salts on deliquescence. In the technical basis document, water chemistries expected in the emplacement drifts caused by seepage water or deliquescence of dust were characterized. The majority of the aqueous solutions are either sulfate or carbonate brines. Effects of initial

water chemistry, relative humidity, and physical processes, such as evaporation, precipitation, and deliquescence, were analyzed. The localized corrosion models for Alloy 22 were developed and are dependent on pH, chloride concentration, nitrate concentration, and temperature. For certain combinations of input parameters, localized corrosion is predicted.

The formation of a calcium chloride brine is modeled with a probability of occurrence of 0.22 percent. Magnesium is not expected to be a component in this type of brine and is expected to precipitate as magnesium silicates. Calcium is expected to precipitate as calcium carbonate. The endpoint of the evaporative concentration of calcium chloride brines is expected to contain significant concentrations of nitrate and sodium.

The DOE assessment of conditions necessary for aqueous solution formation from salts has been revised and incorporates the effects of mixed salts on deliquescence. The deliquescence behavior of mixed salts is included in Bechtel SAIC Company, LLC (2003b). Composition of aqueous solutions from the deliquescence of dust is included in Bechtel SAIC Company, LLC (2003c). Although the supporting analysis/model reports are not publicly available, the Technical Basis Document provides a description of the revised DOE approach.

### 3.2 Agreements Pertaining to Uncertainty and Variability in the Near-Field Geochemical Environment [GEN 1.01 (Comments 93, 98, and 110)]

#### GEN 1.01 (Comment 93) (Reamer, 2001b)

Page 3F-43: Chloride reaches 100,000 mg/L for an extent of 200 m. Wouldn't sorption be potentially a lot different here, compared to ambient chemistry? What about carrier plume effects?

Appendix B of the DOE Technical Basis Document (Bechtel SAIC Company, LLC, 2003a) provides information about GEN 1.01, Comment 93 pertaining to the characteristics (e.g., temperature, density, ionic strength, and pH) of the radionuclide-transporting fluid that are different from those of the ambient fluids, particularly those characteristics affecting sorption. Sorption is dependent on many factors, including temperature, ionic strength, and competition between ions for sorption sites. It is stated in the technical basis document that sorption coefficients used in radionuclide transport models under ambient conditions (Bechtel SAIC Company, LLC, 2003d, Attachment I) were determined from laboratory experiments using the UE p#1 water chemistry (with a higher ionic strength than J-13 Well Water and a chloride concentration of as much as 130 mg/L) as an end-member composition to bracket the impact of water composition on sorption coefficients. Further, simulated high chloride concentrations in Bechtel SAIC Company, LLC (2001, Figure 3.3.6-5) are the result of evaporation, leaving the surroundings quite dry. DOE concludes, for practical purposes, at such locations where chloride concentrates as a result of evaporation, any radionuclide initially dissolved in fracture water would become effectively immobilized, sorption would be largely irrelevant, and its transport would be significantly limited in that region.

GEN 1.01 (Comment 98) (Reamer, 2001b)

Page 4F-34: It is not obvious that the results shown on this page demonstrate good predictability.

Appendix B of the DOE Technical Basis Document (Bechtel SAIC Company, LLC, 2003a) provides DOE responses to GEN 1.01, Comment 98. The comment is related to NRC concerns about the apparent inadequate agreement between results of the DOE thermal-hydrological-chemical model and Drift-Scale Test data. In the technical basis document, it is stated that data from the Drift-Scale Test used for comparison with model results consist of (i) analyses of water and gas samples from borehole intervals between packers (hydrology boreholes) and (ii) observations of mineral precipitation in boreholes (rock samples obtained from rock side-coring). It is stated that differences between the Drift-Scale Test thermal-hydrological-chemical model predictions and the Drift-Scale Test measurements are important to this validation and that observations may disagree with predictions for several reasons and yet are consistent with validation of the Drift-Scale Test thermal-hydrological-chemical model. These reasons include (i) the Drift-Scale Test thermal-hydrological-chemical model is a continuum model, using average hydrologic, thermal, and mineralogical properties for individual hydrostratigraphic units at Yucca Mountain; (ii) the continuum model does not simulate individual fractures; (iii) all samples were taken from long borehole intervals; (iv) the model represents a two-dimensional slice taken approximately at mid-length of the Drift-Scale Test and does not simulate transport in the third dimension; (v) the model does not consider all deviations from planned operation, such as the exact time periods of power losses, variations or uncertainty in heat losses through the bulkhead, changes in pressure owing to forced ventilation, the effect of the many boreholes on the behavior of the system, and barometric pressure changes; and (vi) gas and water samples are affected by condensation of water vapor as the sample cools in the collection tubes from the borehole interval to the sample containers. Thus, DOE concludes that model results cannot be expected to exactly replicate measured data and that the model predictions are reasonable.

GEN 1.01 (Comment 110) (Reamer, 2001b)

Page 6T-1: Capillary pressure effect on chemical potentials of reacting species. It is unclear how this is taken into account because calibration of thermodynamic data result in reproduction of ambient water compositions. The ambient pore waters are at high saturations, which result in relatively low capillary forces. When the rock dries out, the capillary forces may become extremely large. Therefore, it would appear that a calibrated model for a given state of the system is being argued to address an uncertainty for which the calibrated model is likely not valid.

Appendix B of the DOE Technical Basis Document (Bechtel SAIC Company, LLC, 2003a) provides the DOE response to GEN 1.01, Comment 110 pertaining to capillary pressure effect on the chemical potentials of reacting species. DOE states that the effect of capillary pressure on chemical potentials of reacting species is not treated directly but taken indirectly into account through adjustments of thermodynamic data so ambient water compositions can be reproduced. The effect of capillary pressure would be larger in the rock matrix upon

near-complete dryout than during ambient conditions. In addition, most of the fluid transport takes place in fractures where the capillarity is minimal and the potential for water–rock interactions and fluid movement is stronger in zones of large liquid saturations (reflux zone) than in nearly dried-out areas (thus, during liquid saturation/capillary pressure conditions closer to those in the ambient system than in the nearly dry system). Thus, the DOE states the uncertainty resulting from not considering capillary pressure effects on the chemical potential of reacting species should not have a significant impact on predicted seepage water compositions considering the low mobility of waters at low residual saturation in the rock matrix.

### 3.3 Agreements Pertaining to the Modeling of Salt Interactions at Low Relative Humidity [ENFE 2.09 and 2.15]

#### ENFE 2.09 (Reamer, 2001c)

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.

#### ENFE 2.15 (Reamer, 2001c)

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 deliquescence 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.

Appendix F of the DOE Technical Basis Document (Bechtel SAIC Company, LLC, 2003a) provides information about agreements ENFE 2.09 and 15. These agreements are related to NRC concerns about the lack of sufficient technical basis for (i) the low relative humidity salts model, and (ii) the use of sodium nitrate to determine the critical deliquescence relative humidity of salts that may be present on the drip shield and waste package surface.

DOE states that the low relative humidity model, as referred to in the Key Technical Issue agreements no longer is being used by DOE. Instead, a revised model based on the Pitzer ion-interaction approach has been developed and is used by DOE in modeling salt interactions for

the full range of relative humidity relevant for system analyses. The revised model covers the system Na-K-H-Mg-Ca-Al-Cl-F-NO<sub>3</sub>-SO<sub>4</sub>-Br-CO<sub>3</sub>-SiO<sub>2</sub>-CO<sub>2</sub>-O<sub>2</sub>-H<sub>2</sub>O and is valid in the temperature range of 0 to 125 °C. DOE validated the revised model by comparing values calculated with the model to published data about salt solubility, equilibrium relative humidity, and aqueous concentrations in evaporation and deliquescence tests.

The DOE technical basis document indicates that the previous DOE assumption that pure sodium nitrate bounds the critical relative humidity at which deliquescence could begin no longer is used and no longer is applied to the analyses of the chemical environment on the surfaces of the drip shield and waste package. Instead, several model salt assemblages are now defined as representative of the dust salt assemblage and are used to evaluate possible mixed-salt deliquescence curves (i.e., critical relative humidity versus temperature) that could create water at higher temperature conditions.

The revised model encompasses the major ion chemistry output parameters potentially important for estimating corrosion of metals, colloid stability, degradation of engineered barrier system materials, dust deliquescence, and radionuclide transport. These parameters include pH, ionic strength, the total aqueous concentrations of chemical components, the aqueous concentrations of species that potentially contribute to acid-neutralizing capacity, and mineral precipitation.

#### 3.4 Agreement Pertaining to the Kinetics of Chemical Processes [ENFE 2.11]

##### ENFE 2.11 (Reamer, 2001c)

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.

Appendix H of the DOE Technical Basis Document (Bechtel SAIC Company, LLC, 2003a) provides information related to agreement ENFE 2.11, which is related to NRC concerns about the lack of sufficient technical basis for the treatment of the kinetics of chemical processes in the in-drift geochemical models. DOE acknowledges that reaction kinetics are not addressed explicitly in the models. Several arguments are provided as the technical basis for this approach, including applicability of equilibrium models, approximate treatment of kinetics by suppression of precipitation of slowly reacting minerals, consideration of release rates of metals during corrosion, requirements in performance assessment models for time-independent model abstractions, long time scales of in-drift changes relative to the time scales of some relevant chemical reactions, and rapid rates of dissolution of phases originally precipitated during

evaporation of seepage water. DOE includes examples of successful equilibrium modeling of deliquescence and partially successful equilibrium modeling of J-13 Well Water evaporation experiments similar to those by Gdowski (2001), which are referenced in the original agreement.

The technical basis document also clarifies DOE recognition of principal limitations resulting from the lack of explicit treatment of kinetics. For example, equilibrium models may fail to represent accurately supersaturation with respect to minerals that contain corrosive agents. In particular, models that do not represent kinetic precipitation of a fluoride-containing phase could underestimate concentrations of aqueous fluoride, which is potentially a corrosive agent. DOE states that full consideration of water compositions formed by kinetically controlled reaction paths could expand the range of compositions that need to be included in corrosion tests. Also, DOE acknowledges that kinetics should be considered relative to the flow rate of seepage along the drip shield or waste package. Difficulties in modeling evaporation experiments are possibly caused by kinetic effects although uncertainties in thermodynamic parameters are also cited for their possible contributions to discrepancies between models and experimental results.

#### 4.0 NRC EVALUATION AND COMMENT

The following sections provide a discussion of the relevance of the agreements to repository performance followed by results of the NRC review of the agreement responses. The agreements are grouped according to similarity in the aspect of in-drift chemical environment being addressed. The NRC review used the applicable review methods in the Yucca Mountain Review Plan (NRC, 2003).

#### 4.1 Agreements Pertaining to Credible Range of Brine Water Chemistry and Consistency Between Corrosion Testing Environments and Models [TSPAI 3.13 and GEN 1.01 (Comments 50, 113, and 118)]

##### 4.1.1 Relevance to Repository Performance

Waste package and drip shield performances will be affected by the chemistry of water entering the emplacement drifts and the evolution of the water chemistry that contacts the engineered barrier system components. Formation of an aggressive chemistry on the surface of the waste packages and drip shields can promote accelerated degradation modes, such as localized corrosion or enhanced uniform corrosion, as a result of loss of passivity. Characteristics of the environment and water chemistry in contact with the waste package and drip shield that will influence performance include the concentrations of aggressive species, inhibitors, and oxidants, as well as pH, ionic strength, and temperature. Consistency between the environments used in the materials corrosion testing program and the expected environmental conditions that will exist on the waste package and drip shield surfaces is essential to demonstrate an adequate understanding of the corrosion processes and confidence in the barrier performance models.

In the absence of environmental and electrochemical conditions leading to localized forms of corrosion, the drip shield and the waste package will exhibit general corrosion when in contact with an aqueous solution. From general corrosion rate measurements, it has been estimated that the drip shield and waste package lifetimes exceed thousands of years. In the absence of other degradation modes (e.g., localized forms of corrosion and degradation because of

mechanical interactions), the lifetime of these engineered barrier system components is determined by general corrosion rates. Therefore, an appropriate definition of general corrosion rates, their dependence on environmental conditions, and their uncertainty should be considered to radionuclide containment and repository performance.

#### 4.1.2 Data and Model Justification

The TSPAI 3.13 agreement resulted from a staff review of DOE documentation consistent with Review Method 2 in Section 2.2.1.3.1.1 of the Yucca Mountain Review Plan (NRC, 2003). The staff review of the response also was conducted in accordance with the aforementioned review method. This review method requests an evaluation of the sufficiency of experimental and site characterization data to support parameters in conceptual models, process-level models, and alternative conceptual models considered in the total system performance assessment abstraction of degradation of engineered barriers. It also requests the reviewer to verify whether sufficient data have been collected to model adequately degradation processes and confirm that data used to support the total system performance assessment abstraction of the degradation of engineered barriers are based on appropriate techniques and are adequate for sensitivity/uncertainty analyses.

Agreement TSPAI 3.13 focused on the lack of justification for the selection of environments in the Long-Term Corrosion Test Facility used to define general corrosion rates. In the Technical Basis Document, DOE provided rationale for the selection of water chemistries used in the Long-Term Corrosion Test Facility by comparing test solutions to predicted environments. Based on information in the TBD, the staff concludes that considered environments in the Long-Term Corrosion Test Facility support the definition of general corrosion rates in the total system performance assessment abstraction.

GEN 1.01, Comments 50, 113, and 118 resulted from a staff review of DOE documentation consistent with Review Method 2 in Section 2.2.1.3.3.2 of the Yucca Mountain Review Plan (NRC, 2003). The staff review of the response also was conducted in accordance with the aforementioned review method. Review Method Number 2 requests (i) an evaluation of the sufficiency of the models and data used to support the parameters in the abstraction of quantity and chemistry of water contacting the engineered barriers; (ii) an evaluation of whether the basis for the data included a combination of techniques such as laboratory experiments and process-level modeling studies, assessment of how the data were used, interpreted, and synthesized into the parameters; and (iii) verification that sufficient data were collected about the characteristics of the natural system and engineered materials to establish initial and boundary conditions.

GEN 1.01, Comments 50, 113, and 118 focused on the lack of sufficient information on the (i) probability of environmental conditions necessary for localized corrosion, (ii) formation of calcium-magnesium-chloride rich water from pore water, and (iii) effect of mixed salts on deliquescence. Based on the information presented in the Technical Basis Document, DOE has provided sufficient information on the probability of environmental conditions necessary for localized corrosion, formation of calcium-magnesium-chloride rich water from pore water, and the effect of mixed salts on deliquescence.

## 4.2 Agreements Pertaining to Uncertainty and Variability in the Near-Field Geochemical Environment [GEN 1.0 (Comments 93, 98, and 110)]

### 4.2.1 Relevance to Repository Performance

The adequate quantification of uncertainty relative to the development of the seepage water chemistries and constituents that can be present in the in-drift environment is important so engineered barrier performance can be adequately represented at the process model level. The agreement is relevant to repository performance because the abstraction of drift-scale coupled processes is directly used in the total system performance assessment for simulating processes such as engineered barrier degradation and radionuclide mobilization. Therefore, the uncertainty and variability in the abstraction of the seepage chemistry entering the drift should be adequately represented.

### 4.2.2 Model Integration

Issues related to the DOE description of processes affecting radionuclide release from the emplacement drifts discussed in the response to GEN 1.01, Comment 93 are included in the integrated subissue for radionuclide release and solubility limits. The agreement GEN 1.01, Comment 93 resulted from a staff review of DOE documentation that is consistent with Review Method 1 in Section 2.2.1.3.4.2 of the Yucca Mountain Review Plan (NRC, 2003). The staff review of the response also was conducted in accordance with the aforementioned review method. This review method requests verification that the DOE description of conceptual and mathematical models is sufficiently complete with respect to thermal-hydrological processes affecting radionuclide release from the emplacement drifts and an examination of how features, events, and processes related to radionuclide release rates and solubility limits have been included in the total system performance assessment abstraction of radionuclide release rates and solubility limits.

GEN 1.01, Comment 93 is related to NRC concerns about the lack of sufficient technical basis for excluding the effect of ionic strength on the sorption of radionuclides and their release from the near field. In the technical basis document, DOE provided a technical basis for neglecting this effect (see the preceding Section 3.2). Based on a staff review of the DOE response to GEN 1.01, Comment 93, in accordance with methods discussed in the appropriate section of the Yucca Mountain Review Plan (Section 2.2.1.3.4.2, Review Method 1), DOE has provided information requested by the agreement.

Issues related to the DOE model calibration discussed in the response to GEN 1.01, Comment 110 are included in the integrated subissue for quantity and chemistry of water contacting engineered barriers and waste forms. GEN 1.01, Comment 110 resulted from a staff review of DOE documentation that is consistent with Review Method 1 in Section 2.2.1.3.3.2 of the Yucca Mountain Review Plan (NRC, 2003). The staff review of the response also was conducted in accordance with the aforementioned review method. This review method requests an examination of the descriptions of physical phenomena and couplings included in the abstraction of quantity and chemistry of water contacting engineered barriers and waste forms. The review method also asks for an examination of how the features, events, and processes related to the quantity and chemistry of water contacting engineered barriers and waste forms have been included in the total system performance assessment abstraction.

GEN 1.01, Comment 110 is related to NRC concerns about the lack of sufficient technical basis for excluding capillary pressure effect on the chemical potentials of reacting species in the DOE thermal-hydrological-chemical models. In the technical basis document, DOE provided technical bases for neglecting this effect (see the preceding Section 3.2). Based on a staff review of the DOE response to GEN 1.01, Comment 110, in accordance with methods discussed in the appropriate section of the Yucca Mountain Review Plan (Section 2.2.1.3.3.2, Review Method 1), DOE has provided the information requested by the agreement.

#### 4.2.3 Data and Model Justification

GEN 1.01, Comment 98 resulted from a staff review of DOE documentation consistent with Review Method 2 in Section 2.2.1.3.3.2 of the Yucca Mountain Review Plan (NRC, 2003). The staff review of the response also was conducted in accordance with the aforementioned review method. This review method requests evaluation of the sufficiency of geological, hydrological, and geochemical data to support parameters in conceptual models, process-level models, and alternative conceptual models considered in the abstraction of quantity and chemistry of water contacting engineered barriers and waste forms. It also requests the reviewer to verify whether sufficient data have been collected to support thermal-hydrological conceptual models.

GEN 1.01, Comment 98 is related to NRC concerns about the apparent lack of agreement between results of the DOE thermal-hydrological-chemical model and Drift-Scale Test data. In the technical basis document, DOE provided technical bases for this apparent lack of agreement (see the preceding Section 3.2). Based on a staff review of the DOE response to GEN 1.01, Comment 98, in accordance with methods discussed in the appropriate section of the Yucca Mountain Review Plan (Section 2.2.1.3.3.2, Review Method 2), the response provides the information requested by the agreement.

#### 4.3 Agreement Pertaining to the Modeling of Salt Interactions at Low Relative Humidity [ENFE 2.09 and 2.15]

##### 4.3.1 Relevance to Repository Performance

Evaporation of seepage water can have a significant effect on the chemistry of water that contacts the drip shield and waste package. Initially dilute seepage water can become a corrosive brine upon evaporation, so the performance of the engineered barriers potentially can diminish. Corrosive brines also could form from deliquescence of dusts and salts in the repository drift. Prediction of the chemical evolution—caused by evaporation, mineral precipitation, and deliquescence—of water that contacts the drip shield and waste package is necessary to evaluate the impact of those processes on the performance of the engineered barriers.

##### 4.3.2 Data and Model Justification

Issues related to the DOE in-drift precipitates/salts model discussed in the response to ENFE 2.09 and 2.15 are included in the integrated subissue for quantity and chemistry of water contacting engineered barriers and waste forms. The ENFE 2.09 and 2.15 agreements resulted from a staff review of DOE documentation consistent with Review Method 2 in Section 2.2.1.3.3.2 of the Yucca Mountain Review Plan (NRC, 2003). The staff review of the response also was conducted in accordance with the aforementioned review method. This review method

requests an evaluation of the sufficiency of the geochemical data used to support the parameters in the in-drift precipitates/salts model, an evaluation of whether the basis for the data included a combination of techniques, such as laboratory experiments and process-level modeling studies, and an assessment of how the data were used, interpreted, and synthesized into the parameters.

The KTI Agreements, ENFE 2.09 and 2.15, focused on the lack of sufficient technical basis for (i) the low relative humidity salts model, and (ii) the use of sodium nitrate to determine the critical deliquescence relative humidity of salts that may be present on the drip shield and waste package surface. Based on information presented in the Technical Basis Document, DOE has improved the in-drift precipitates/salts model, and the low relative humidity model used in previous DOE analyses no longer is used. Validation of the revised model was demonstrated by the agreement between calculated values and a variety of experimental data. In addition, the assumption that sodium nitrate bounds the critical deliquescence relative humidity of salts that may be present on the drip shield and waste package surface no longer is used in the DOE analyses. Based on the staff review of the DOE response to ENFE 2.09 and 2.15, in accordance with methods discussed in the appropriate section of the Yucca Mountain Review Plan (Section 2.2.1.3.3.2, Review Method 2), the DOE response provides the information requested by the agreements.

#### 4.4 Agreement Pertaining to the Kinetics of Chemical Processes [ENFE 2.11]

##### 4.4.1 Relevance to Repository Performance

Kinetics of chemical reactions among groundwater and components of the in-drift environment can have a significant effect on the chemistry of water that contacts the drip shield and waste package. In turn, water chemistry can affect rates of engineered barrier degradation, release rates of radionuclides, concentration limits of released radionuclides, and radionuclide transport processes. Ultimately, the performance of engineered barriers may depend on rates of in-drift chemical reactions. In general, rapid reaction rates (fast kinetics) lead to conditions of chemical equilibrium. Equilibrium models are conservative relative to kinetic models with respect to many aspects of repository performance at Yucca Mountain because of the thermodynamic instability of engineered barrier components including waste forms. For some processes, however, slow kinetic controls on in-drift chemical reactions could adversely affect performance. Such cases include slow precipitation of a solid phase permitting elevated concentrations of a corrosive agent relative to equilibrium concentrations and slow precipitation of a radionuclide solubility controlling solid phase.

##### 4.4.2 Data and Model Justification

Issues related to the DOE in-drift kinetics of chemical processes discussed in the response to ENFE 2.11 are included in the integrated subissue for quantity and chemistry of water contacting engineered barriers and waste forms. The ENFE 2.11 agreement resulted from a staff review of DOE documentation consistent with review methods in Section 2.2.1.3.3.2 of the Yucca Mountain Review Plan (NRC, 2003). The staff review of the response also was conducted in accordance with the aforementioned review methods. This review method requests an evaluation of the sufficiency of the data used to support parameters in the in-drift kinetics model, an evaluation of whether the basis for the data included a combination of techniques such as laboratory experiments and process-level modeling studies, and an assessment of how the data were used, interpreted, and synthesized into the parameters.

The KTI agreement ENFE 2.11 focuses on the technical basis for the treatment of the kinetics of chemical processes in the in-drift geochemical models. Based on information presented in the Technical Basis Document (Bechtel SAIC Company, LLC, 2003a), DOE has provided a technical basis for assumptions in its in-drift chemical models that do not explicitly treat chemical kinetics. The basis for this approach includes the applicability of equilibrium models caused by long time scales and rapid reactions, the approximate treatment of kinetics by suppression of precipitation of certain phases, and consideration of rates of corrosion. In addition, arguments are offered that time-independent (i.e., not kinetic) abstractions of chemical conditions are required for use in performance assessment modeling. Furthermore, in the technical basis document, DOE provides clear recognition of the limitations of models that neglect kinetics of in-drift chemical processes and of the potentially adverse consequences of these assumptions in assessments of repository performance.

Based on the staff review of the DOE response to ENFE 2.11, in accordance with methods discussed in the appropriate section of the Yucca Mountain Review Plan (Section 2.2.1.3.3.2, Review Method 2), the DOE response provides the information requested by the agreement.

## 5.0 SUMMARY

NRC reviewed the DOE KTI Agreement responses within the Technical Basis Document to determine whether sufficient information was provided to close the agreement items. On the basis of this review and notwithstanding new information that could raise new questions or comments concerning the above agreements, DOE has provided the information requested in agreements ENFE 2.09, 2.11, and 2.15, TSPAI 3.13, and GEN 1.01, Comments 50, 93, 98, 110, 113, and 118.

## 6.0 STATUS OF THE AGREEMENTS

Based on the above review, NRC considers the agreements ENFE 2.09, 2.11, and 2.15, TSPAI 3.13, and GEN 1.01, Comments 50, 93, 98, 110, 113, and 118 complete.

## 7.0 REFERENCES

Bechtel SAIC Company, LLC. "Technical Basis Document No. 5: In-Drift Chemical Environment." Rev. 1. Las Vegas, Nevada: Bechtel SAIC Company, LLC. 2003a.

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——— "U.S. Nuclear Regulatory Commission/U.S. Department of Energy Technical Exchange and Management Meeting on Range of Thermal Operating Temperatures (September 18–19, 2001)." Letter (October 2, 2001) to S. Brocoum, DOE. Washington, DC: NRC. 2001b.

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