

REVIEW BY THE NUCLEAR REGULATORY COMMISSION  
OFFICE OF NUCLEAR MATERIAL SAFETY AND SAFEGUARDS  
OF THE DEPARTMENT OF ENERGY AGREEMENT RESPONSES RELATED TO THE  
POTENTIAL GEOLOGIC REPOSITORY AT YUCCA MOUNTAIN, NEVADA:  
IN-DRIFT CHEMICAL ENVIRONMENT-RELATED AGREEMENTS  
FOR KEY TECHNICAL ISSUES “CONTAINER LIFE AND SOURCE TERM” (CLST 1.01),  
“EVOLUTION OF THE NEAR-FIELD ENVIRONMENT” (ENFE 2.04, 2.14),  
AND “GENERAL” (GEN 1.01, COMMENTS 122, 124)

## 1.0 INTRODUCTION

The U.S. Nuclear Regulatory Commission (NRC) issue resolution goal during this interim precicensing period is to ensure that the U.S. Department of Energy (DOE) has assembled sufficient information about a given issue for NRC to begin review of a potential license application. Resolution by NRC during precicensing 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 precicensing period is only a determination that it appears sufficient information will be available to review a potential license application, and does not prejudice the outcome of an NRC evaluation of the issue during a potential licensing review. Issues are resolved by NRC during precicensing when the staff have 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 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 (Schlueter, 2000), January 2001 (Reamer, 2001a), August 2001 (Reamer, 2001b), and September 2001 (Reamer, 2001c). The specific agreements addressed in the technical basis document are categorized according to five different key technical issues:

- (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 should be considered complete. Section 4.0 of this report provides the NRC evaluation of the

extent to which the DOE submittal satisfies three of the agreements (CLST 1.01, ENFE 2.04, 2.14) and two of the GEN 1.01 Comments (122 and 124). In a previous letter, NRC indicated that the responses provided by the DOE in Bechtel SAIC Company, LLC (2003a) satisfy the agreements ENFE 2.09, 2.11, 2.15, and TSPAI 3.13, and the GEN 1.01 Comments 50, 93, 98, 110, 113, and 118. NRC evaluation of the extent to which the DOE submittal satisfies agreement TSPAI 3.12 will be provided in a separate letter documenting NRC evaluation of DOE information provided in the report titled "Technical Basis Document No. 6: Waste Package and Drip Shield Corrosion" (Bechtel SAIC Company, LLC, 2003b). Evaluation of whether DOE satisfied the other agreements will be provided in a separate document.

## 2.0 WORDING OF THE AGREEMENTS

In Appendixes A, C, and J of Technical Basis Document No. 5, DOE identified the following key technical issue agreements as being satisfied by the information provided in the report. The wording of the agreements, grouped according to similarity in the aspect of in-drift chemical environment being addressed, is listed in the following three subsections.

### 2.1 Agreements Pertaining to Credible Range of Brine Water Chemistry and Consistency Between Corrosion Testing Environments and Models [CLST 1.01 and GEN 1.01 (Comments 122 and 124)]

#### CLST 1.01

The agreement reads (Schlueter, 2000):

"Provide the documentation for Alloy 22 and titanium for the path forward items listed on slide 8 [establish credible range of brine water chemistry; evaluate effect of introduced materials on water chemistry; determine likely concentrations and chemical form of minor constituents in YM waters; characterize YM waters with respect to the parameters which define the type of brine which would evolve; evaluate periodic water drip evaporation]. DOE will provide the documentation in a revision to AMR "Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier" by LA."

#### GEN 1.01 (Comment 122)

The agreement reads (Reamer, 2001b):

"In p. 7-58, fluoride mitigates corrosion. Provide the basis for this mitigation."

#### GEN 1.01 (Comment 124)

The agreement reads (Reamer, 2001b):

"In p. 7-74, Ferric chloride generation is very remote spatially. Provide the basis for the hypothesis."

## 2.2 Agreement Pertaining to Evaluation of Trace Elements and Fluoride (ENFE 2.04)

The agreement reads (Reamer, 2001a):

“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–EBSMD–000033), expected to be available in FY 02.”

## 2.3 Agreement Pertaining to the Analysis of Laboratory Solution of Introduced Materials (ENFE 2.14)

The agreement reads (Reamer, 2001a):

“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.”

## 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 [CLST 1.01 and GEN 1.01 (Comments 122 and 124)]

#### CLST 1.01

Appendix A of the DOE technical basis document (Bechtel SAIC Company, LLC, 2003a) provides information related to agreement CLST 1.01. This agreement requests DOE to provide documentation supporting its analysis of the credible range of brine water chemistry that may contact the drip shields and waste packages, the effect of introduced materials on water chemistry, the likely concentrations and chemical form of minor constituents in Yucca Mountain waters, the type of brines that could evolve from Yucca Mountain waters, and the effect of periodic water drip evaporation. Chemical conditions on the drip shield and waste package surfaces are established by the chemistry of water leaving the host rock as modified by reactions with drift support materials and in-drift gases and by evaporation from warmer drip shield and waste package surfaces.

As discussed in the technical basis document, DOE determined a credible range of brine water chemistry on the drip shield and waste package surfaces by establishing a credible range of dilute water chemistries that may seep through Yucca Mountain and by modeling the evolution of these waters under repository relevant conditions. The seepage water compositions were

modeled using the Drift-Scale Coupled Processes (DST and THC Seepage) Models (Bechtel SAIC Company, LLC, 2003c), based on five water compositions selected to represent the spread of potential porewater compositions. The In-Drift Precipitates/Salts Model (Bechtel SAIC Company, LLC, 2003d) was used to determine the chemical evolution of representative water compositions selected from the thermal-hydrological-chemical seepage model outputs in response to evaporation caused by a combination of decreasing relative humidity and (or) increasing temperature. The large number of calculated water chemistries from the thermal-hydrological-chemical model was abstracted by grouping them into 11 water types (bins) that yield carbonate-, sulfate-, and calcium chloride-type brines after they are concentrated by evaporation. Dust leachate waters extracted from dust samples collected at the Exploratory Studies Facility were binned using a similar process to produce six likely compositions for brines formed by deliquescence of salt dusts.

DOE evaluated the potential impact of the corrosion of introduced materials—stainless and carbon steels used as ground support materials—on the composition of seepage waters. The analysis was done by thermodynamic simulation of titration of a solution with dissolved iron and chromium, representative of Type 316 stainless steel, into a typical seepage water. The seepage water was a dilute, near-neutral water believed to represent a likely seepage water composition. The calculations showed little impact of the corrosion of stainless steel Type 316 wire mesh and rock bolts on the seepage water composition. The results were expected because the corrosion products (iron, nickel, and chromium oxides and hydroxides) have very low solubility in the dilute near-neutral waters.

Minor constituents, such as lead, mercury, and arsenic, in waters that contact the engineered barrier system components may enhance the degradation of those components. The likely presence and potential impact of these minor constituents on the in-drift chemical environmental conditions were evaluated by DOE and discussed in the technical basis document (Bechtel SAIC Company, LLC, 2003a). Dissolved lead concentrations in groundwater are believed to be controlled by lead adsorption on mineral surfaces and organic matter, as well as by precipitation of lead minerals (e.g., carbonates, sulfides, and phosphates). Based on literature studies of other waters containing minerals found at Yucca Mountain (e.g., smectite, illite, zeolites, glass, and cristobalite), DOE stated that sorption of lead to mineral surfaces will be important in limiting lead concentration in groundwater at Yucca Mountain. Ambient Yucca Mountain groundwater mercury concentrations are expected to be quite low, between  $10^{-2}$  and  $10^{-3}$  ppb. Although mercury has few solubility controls, DOE stated that the ability of mercury to concentrate in brine water is limited because it is volatile and transfers to the atmosphere, especially at the elevated temperatures anticipated in the repository environment. The concentration of arsenic in repository water likely will increase as the groundwater evaporates and as arsenic present in the volcanic glass dissolves. DOE stated that a limitation on the amount of dissolved arsenic will be the dissolution of the volcanic glass that is the source of the arsenic.

DOE discussed the parameters and processes that control the evolution of the environment on the waste package and drip shields. These parameters and processes include the geology and geochemistry at Yucca Mountain, the environmental conditions (e.g., temperature and relative humidity) at the engineered barrier system components, the partial pressures of acid gases that influence the chemistry of the aqueous solutions, and physical separation and fractionation that can change the compositions of water.

DOE evaluated periodic water drip evaporation based on the work of Drever (1997), who assessed the effect of cyclic wetting and drying on aqueous solution chemistry. DOE concluded that wetting and drying cycles primarily affects the less soluble aqueous species and that water chemistries resulting from wetting and drying cycles are predictable based on thermodynamics.

#### GEN 1.01 (Comment 122)

Appendix A of the DOE technical basis document (Bechtel SAIC Company, LLC, 2003a) provides information about GEN 1.01, Comment 122, which is related to NRC concerns about the lack of information on the technical basis for the DOE statement that fluoride mitigates corrosion. It is stated in the technical basis document that literature and DOE Yucca Mountain Project data show that fluoride has an accelerating effect on the degradation of titanium-based alloys, although the DOE analysis shows that the presence of fluoride will not significantly enhance the general corrosion of the drip shield material and will not limit the lifetime of titanium alloys in repository environments. DOE also states that Alloy 22 does not suffer localized corrosion in fluoride-only solutions and no localized corrosion of Alloy 22 has been observed in multi-ionic solutions containing fluoride.

#### GEN 1.01 (Comment 124)

Appendix A of the DOE technical basis document (Bechtel SAIC Company, LLC, 2003a) provides information about GEN 1.01, Comment 124, which is related to NRC concerns about the lack of information on the technical basis for the DOE hypothesis that ferric chloride is not present in significant quantity. The effect of ferric chloride on engineered barrier system component corrosion is to raise the corrosion potential (ferric ions are oxidizing) in acidic chloride aqueous solutions. DOE believes that aqueous ferric chloride solutions will not be stable during relevant repository conditions, even though ferric ions could be formed by corrosion of ground support materials. Ferric ions are stable in aqueous solutions lower than pH Three and oxidizing conditions. In the technical basis document, DOE stated that the low pH necessary to stabilize the ferric ions is not expected under repository conditions.

### 3.2 Agreement Pertaining to Evaluation of Trace Elements and Fluoride (ENFE 2.04)

#### ENFE 2.04

Appendix C of the DOE technical basis document (Bechtel SAIC Company, LLC, 2003a) provides information related to agreement ENFE 2.04. This agreement is related to NRC concerns about the lack of information on the technical basis for bounding the concentrations of trace elements and fluoride in waters that may contact and possibly enhance the corrosion of the drip shields and waste packages. In the technical basis document, DOE evaluated the presence of minor and trace elements, specifically fluoride, bromide, and lead, and their potential to directly affect an engineered barrier in the engineered barrier system. Fluoride was included explicitly in the DOE model predicting the constituents for the evaporated seepage or deliquescent water. Fluoride concentrations approaching 1 molal were calculated to form, but DOE concluded that a high concentration of fluoride ions will not significantly enhance the general corrosion of drip shield material under the repository conditions. The DOE model showed also that bromide ions tend to concentrate during evaporation. Lead initially was considered by DOE as a possibly aggressive trace element based on experiments conducted by Catholic University of America (Pulvirenti, et al., 2002). Lead has been included in certain

DOE waste package corrosion testing environments, with no observed impact on stress corrosion cracking. In Appendix C, DOE assumed that lead adequately represents other trace elements such as arsenic and mercury relative to waste package corrosion processes, and separate evaluations pertaining to these other trace elements were not provided in Appendix C. Additional discussion was provided in Appendix A regarding the issues of lead, mercury, and arsenic content in natural waters and phenomena that may limit their aqueous concentrations.

### 3.3 Agreement Pertaining to the Analysis of Laboratory Solution of Introduced Materials (ENFE 2.14)

#### ENFE 2.14

Appendix J of the DOE technical basis document (Bechtel SAIC Company, LLC, 2003a) provides information related to agreement ENFE 2.14. This agreement is related to NRC concerns about the lack of information on the concentration of minor and trace elements that could be derived from interaction of in-drift water with introduced materials. NRC was concerned about the potential effect of these minor and trace constituents on the degradation of the engineered barriers. For example, experiments conducted by Catholic University of America (Pulvirenti, et al., 2002) appeared to show that trace constituents such as lead could enhance the corrosion of the waste package material.

The DOE response provided in Appendix J consisted primarily of computer simulation, instead of laboratory analysis as called for in the text of agreement ENFE 2.14. The computer simulation focused on the stainless steel components and their corrosion and utilizes published rates of corrosion and materials composition used in the engineered barrier system. DOE concluded that stainless steel corrosion is likely to have only a very minor effect on seepage water chemistry. No results were provided in Appendix J for possible concentration of trace constituents such as lead, mercury, or arsenic, although discussions pertaining to these trace constituents were provided in Appendixes A and C.

## 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 [CLST 1.01 and GEN 1.01 (Comments 122 and 124)]

#### 4.1.1 Relevance to Repository Performance

Understanding the in-drift environment is important because it directly impacts waste package and drip shield performance. The environmental conditions that the waste package and drip shield are subjected to and the evolution of the water chemistry play a substantial role in determining the potential for corrosion of these engineered barriers. A consistency between the environment used in the materials corrosion testing program and the environment that is

expected to exist on the waste package and drip shield surfaces is essential to demonstrate adequately the understanding and development of the barrier performance models. Discrepancies between corrosion testing environments and expected repository environments can impact estimation of the lifetime of engineered barriers.

#### 4.1.2 Model Integration

The CLST 1.01 agreement resulted from a staff review of DOE documentation consistent with Review Method 1 in Section 2.2.1.3.1.2 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 adequacy of DOE descriptions of aspects of environmental conditions, within the waste package emplacement drifts, design features, physical phenomena, and couplings that may affect the degradation of the engineered barriers. Agreement CLST 1.01 focused on the lack of information on the technical basis for the DOE analysis of the credible range of brine water chemistry that may contact the drip shields and waste packages. Further, the intent of this agreement was to obtain an understanding of the process and the logic that the DOE used to develop the range of chemistries that might contact the drip shield or waste packages. Specific questions regarding specific chemistries are addressed through other agreements. In the technical basis document, DOE provided its technical bases for the range of brine water chemistry that is expected on the drip shield and waste package surfaces, including an evaluation of the effects of introduced materials and minor constituents, the parameters that define the type of brine that would evolve, and periodic water drip evaporation. Based on information presented in the technical basis document, DOE has provided the documentation requested in agreement CLST 1.01.

GEN 1.01, Comment 122 resulted from a staff review of DOE documentation consistent with Review Method 1 in Section 2.2.1.3.1.2 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 adequacy of DOE descriptions of aspects of environmental conditions, within the waste package emplacement drifts, design features, physical phenomena, and couplings that may affect the degradation of the engineered barriers. GEN 1.01, Comment 122 focused on the lack of information on the technical basis for the DOE statement that fluoride mitigates corrosion. In the technical basis document, it is indicated that DOE no longer sustains the validity of that statement. On the contrary, DOE analysis shows that fluoride has an accelerating effect on the degradation of titanium-based alloys.

GEN 1.01, Comment 124 resulted from a staff review of DOE documentation consistent with Review Method 1 in Section 2.2.1.3.1.2 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 adequacy of DOE descriptions of aspects of environmental conditions, within the waste package emplacement drifts, design features, physical phenomena, and couplings that may affect the degradation of the engineered barriers. GEN 1.01, Comment 124 focused on the lack of information on the technical basis for the DOE hypothesis that ferric chloride is very remote spatially. In the technical basis document, DOE stated that the low pH necessary to stabilize the ferric ions is not expected under repository conditions, although no analysis to support this assertion was provided in the document. The possibility of formation of acidic solutions has been raised by Catholic University of America experiments in which acidic solutions and vapors resulted from

evaporation of an initially dilute porewater similar to those found in the unsaturated zone of Yucca Mountain (Pulvirenti, et al., 2003, 2004). However, there are several processes that will mitigate the formation of these acidic solutions and vapors (Browning, et al., 2004; Pabalan, et al., 2004; Steefel, 2004).

First, acidic gases will not form from initially dilute porewaters unless the porewaters were subjected to very high degrees of evaporation and to high temperatures. Second, acid gases that are formed will disperse rapidly into the drift environment and mix with other gases, mainly water vapor, inside the drift. Third, acidic solutions and gases will be neutralized by interactions with drift wallrocks, ground support materials, in-drift water, and wallrock porewaters. Based on this information, NRC agrees with DOE that the intent of GEN 1.01, Comment 124 has been satisfied.

#### 4.2 Agreement Pertaining to Evaluation of Trace Elements and Fluoride (ENFE 2.04)

##### 4.2.1 Relevance to Repository Performance

Certain minor and trace elements potentially are deleterious to the performance of engineered barrier materials. For example, potentiostatic measurements of the anodic polarization behavior of Titanium Grade 7 in deaerated 1 M NaCl solutions (pH 6.4 to 8.2) at 95 °C [203 °F] indicated that accelerated general corrosion of the titanium alloy occurs when fluoride ion is present at a concentration of approximately 0.0005 M or greater (Brossia, et al., 2001). In experiments by Pulvirenti, et al. (2002) using acidified groundwater solution at 160–250 °C [320–482 °F], the presence of lead or mercury was observed to cause pitting of both U-bend and disk specimens of Alloy 22. An evaluation of trace elements and fluoride in waters that may contact the drip shields and waste packages is important to determine their potential effect on the degradation of these engineered barriers.

##### 4.2.2 Model Integration

The ENFE 2.04 agreement resulted from a staff review of DOE documentation 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 evaluation of the adequacy of DOE descriptions of geochemistry, physical phenomena, and couplings that may affect the chemistry of water contacting engineered barriers and wasteforms. Agreement ENFE 2.04 focused on the lack of information on the technical basis for the range of the concentrations of trace elements and fluoride in waters that may contact and possibly enhance the corrosion of the drip shields and waste packages. In the technical basis document, DOE provided its technical bases for bounding the trace elements and fluoride for the geochemical environment affecting the drip shield and waste package, including the impact of engineered materials. In summary, DOE addressed both minor and trace elements, specifically fluoride, bromide and lead. Other trace elements such as arsenic and mercury were treated as analogs to lead. In general, DOE concluded that trace elements are present in such low abundance that they are unlikely to significantly affect major constituent geochemistry, and therefore are not generally included in the models that determine the geochemistry of the system. Based on information presented in the technical basis document, DOE has provided the technical bases requested in ENFE 2.04.



#### 4.3 Agreement Pertaining to the Analysis of Laboratory Solution of Introduced Materials (ENFE 2.14)

##### 4.3.1 Relevance to Repository Performance

Introduced materials in the repository can impact the evolution of water chemistry within the drift, potentially affecting the performance of the waste package and drip shield. For the purposes of establishing waste package and drip shield degradation rates and performance, it is important to carry out corrosion testing and analyses that are consistent with environmental conditions expected for the repository drift.

##### 4.3.2 Model Integration

The ENFE 2.14 agreement resulted from a staff review of DOE documentation 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 evaluation of the adequacy of DOE descriptions of geochemistry, physical phenomena, and couplings that may affect the chemistry of water contacting engineered barriers and waste forms. Agreement ENFE 2.14 focused on the lack of information on the interaction of in-drift water with introduced materials that may enhance the corrosion of the drip shields and waste packages.

Although the agreement requested the analysis of laboratory solutions that have interacted with introduced materials, the intent of the agreement was to obtain an understanding of the concentration of minor and trace constituents that could be derived from interaction of in-drift water with introduced materials. DOE addressed this topic primarily through computer simulations as opposed to laboratory testing. The material modeled (metallic ground support elements) would be in the flow path between the host rock and the engineered barriers (drip shield and waste package). DOE used corrosion rates and compositional constraints (from industry standards) to model the resulting chemical changes from the release of major components (Fe and Cr) of an introduced material. DOE modeled only Fe and Cr because the other constituents would be present only in trace quantities in the introduced materials. Based on information provided in the technical basis document, DOE has provided an alternate technical basis that satisfies the intent of ENFE 2.14.

#### 5.0 SUMMARY

NRC reviewed the DOE key technical issue 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, NRC considers that the information provided in the technical basis document, together with information from the literature, satisfies the intent of the agreements CLST 1.01, ENFE 2.04, 2.14, and GEN 1.01, Comments 122 and 124.

#### 6.0 STATUS OF THE AGREEMENTS

Based on the above review, NRC agrees with DOE that the information provided satisfies the

intent of the agreements. Therefore, NRC considers the agreements CLST 1.01, ENFE 2.04, 2.14, and General 1.01 (Comments 122 and 124) complete.

## 7.0 REFERENCES

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