COMPLIANCE DETERMINATION STRATEGY
RRT 3.2.3.5 POTENTIALLY ADVERSE CONDITION: GEOCHEMICAL PROCESSES

APPLICABLE REGULATORY REQUIREMENT(S):

10 CFR 60.122(c)(8)
10 CFR 60.21(c)(1)(ii)(B)
10 CFR 60.21(c)(1)(ii)(F)

TYPES OF REVIEW:

Acceptance Review (Type 1)
Safety Review (Type 3)
Detailed Safety Review Supported by Analysis (Type 4)
Detailed Safety Review Supported by Independent Tests, Analyses, or Other Investigations (Type 5)

RATIONALE FOR TYPES OF REVIEW:

Acceptance Review (Type 1) Rationale:

This regulatory requirement topic is considered to be license application-related because, as specified in the license application content requirements of 10 CFR 60.21 and the regulatory guide "Format and Content for the License Application for the High-Level Waste Repository (FCRG)" it must be addressed by the U.S. Department of Energy (DOE) in its license application. Therefore, the staff will conduct an Acceptance Review of the license application for this regulatory requirement topic.

Safety Review (Type 3) Rationale:

This regulatory requirement is considered to be related to containment and waste isolation. It is a requirement for which compliance is necessary to make a safety determination for construction authorization as defined in 10 CFR 60.31(a) (i.e., regulatory requirements in Subparts E, G, H, and I). Therefore, the staff will conduct a Safety Review of the license application to determine compliance with this regulatory requirement topic.

This regulatory requirement topic, concerning a potentially adverse condition (PAC), focuses on geochemical processes that would reduce sorption of radionuclides, result in degradation of rock strength, or adversely affect the performance of the engineered barrier system.

In order to evaluate information concerning the presence or absence of the PAC, the NRC staff had to determine the meaning of the term "geochemical processes." The NRC staff decided to interpret the term "geochemical process" to mean "any process in the repository environment that could affect or be affected by the geochemistry or chemistry of the system. Various geochemical processes, singly or in combination, may lead to potentially adverse geochemical conditions. Some of these geochemical processes are listed in Table 1.

It is recognized that the entries listed in Table 1 include chemical, physical and biological processes. Furthermore, a number of the processes in the table may overlap, as, for example, alteration versus precipitation and dissolution, or sorption versus ion exchange. The emphasis in selecting entries to the

Table 1. Geochemical Processes

precipitation	diffusion	volatilization
dissolution	dehydration	nucleation
sorption	oxidation	anion exclusion
desorption	reduction	osmosis
speciation	hydrolysis	melting
solation	radiolysis	crystallization
gelation	microbial processes	coprecipitation
evaporation	radioactive decay	devitrification
condensation	isotopic fractionation	ion exchange
alteration	radiation damage	Ostwald ripening
flocculation	catalysis	corrosion
dispersion	advection	metasomatism
expansion	contraction	filtration

table was to identify as many processes associated with geochemical reactions as possible with little concern for eliminating potentially inappropriate entries. In that way, there was less chance for a process to be omitted. This list should, however, be considered incomplete as other unidentified processes most likely exist.

The geochemical processes considered in this CDS are those that have occurred in the past, are occurring now, or will occur in the future. Furthermore, processes in the future will include those that apply to perturbation of the site by the repository, and those that occur under unperturbed conditions.

The regulatory requirement topic is concerned with the potentially adverse effect of geochemical processes on three characteristics: 1) sorption of radionuclides, 2) rock strength, or 3) the performance of the engineered barrier system. The use of the word "or" means that the effects on each one of the characteristics must be evaluated individually. Furthermore, a given process can affect each of these characteristics differently. For example, some speciation processes may reduce radionuclide sorption but improve the performance of the engineered barrier system. Thus, the PAC would be present for one characteristic but not for the other. However, if the PAC is present for any of the three characteristics, it is to be considered present.

Some geochemical processes might have opposite effects on the same characteristic (1, 2, or 3 in the preceding paragraph) of the PAC but involving different constituents including radionuclides, different locations in the controlled area, or different times at which the processes are occurring. For example, if different radionuclides are competing for the same ligand, complexation of one radionuclide may make it less likely to be sorbed whereas the competing radionuclide would more likely be sorbed.

To determine whether a PAC is present, DOE will most likely have to consider all processes involving all constituents at all places and all times in the repository out to the accessible environment. This large task, however, can be minimized by considering only those processes and conditions that can have an adverse effect on the performance objectives. Thus it is expected that DOE would initially eliminate from further consideration those processes that either are not expected at Yucca Mountain or would have no effect on the performance objectives.

In parallel with this expectation, the NRC staff has divided the processes in Table 1 into three categories - those that are likely to contribute to the existence of the PAC characteristic, those that are unlikely to contribute to the existence of the PAC, and those whose effect could contribute to the potentially adverse condition or could contribute to a favorable condition depending upon the set of chemical components involved in the process or the conditions in which the process occurs.

Given the complex nature of this regulatory requirement, it is prudent to divide the requirement into its parts and describe the rationale for each separately.

<u>Reduction of radionuclide sorption</u>

Since this regulatory requirement topic describes a potentially adverse condition, it is assumed that processes that would reduce sorption should result in increased radionuclide flux to the accessible environment. However, it is conceivable that some processes, while reducing sorption, may also decrease the radionuclide flux to the accessible environment. For example, precipitation and coprecipitation of radionuclide-bearing phases could reduce radionuclide sorption, while at the same time decreasing radionuclide flux and so their effect would not lead to a potentially adverse condition.

Since the DOE will have to demonstrate that assumptions made in evaluating evidence for this PAC do not minimize its effect, the NRC staff assumes retardation processes other than sorption will be considered by DOE. Coupling this assumption with the fact that some processes can reduce sorption but not lead to a potentially adverse condition, the staff has chosen to interpret the word "sorption" in 10 CFR 60.122(c)(8) to mean "retardation." In that way, "geochemical processes that reduce retardation of radionuclides" will constitute a potentially adverse condition.

It is assumed that these processes are to be considered for the farfield. The contribution of precipitation, crystallization, and nucleation to a reduction in radionuclide retardation is uncertain since the precipitation of a radionuclide could, in most cases, immobilize it, (e.g. DOE, 1988, p. 8.3.1.3-85, SCP Investigation 8.3.1.3.5 Radionuclide retardation by precipitation processes along flow paths to the accessible environment), but in other cases could promote radionuclide mobility. Reardon (1981), for example, showed that the precipitation of a nonradioactive phase could lead to the reduction in sorption of a radionuclide. Thus, it would be expected that DOE will have to demonstrate the effect of precipitation reactions on radionuclide retardation.

Similarly, sorption and ion exchange are listed as likely to contribute to or likely to compensate for reduction in radionuclide retardation depending upon the chemical involved in the process. In most cases, sorption will lead to the retardation of radionuclides. But one can conceive of a situation where the sorption of one species reduces the sorption of another, as in ion exchange. If the sorbed species is nonradioactive, its sorption can reduce that of the competing radionuclide, making it more mobile.

Table 2. Geochemical Processes Potentially Reducing Radionuclide Retardation*

precipitation	£	diffusion	£	volatilization	L
dissolution	£	dehydration	£	nucleation	U
sorption	£	oxidation	L	anion exclusion	L
desorption	£	reduction	U	osmosis	U
speciation	£	hydrolysis	£	melting	U
solation	L	radiolysis	L	crystallization	U
gelation	L	microbial processes	L	coprecipitation	U
evaporation	U	radioactive decay	U	devitrification	U
condensation	U	isotopic fractionation	U	ion exchange	£
alteration	£	metamictization	U	Ostwald ripening	U
flocculation	£	catalysis	£	corrosion	L
expansion	U	contraction	U	filtration	U

*U = process is considered unlikely to contribute to PAC
L = process is considered likely to contribute to PAC
£ = process is considered likely to affect (i.e., contribute to or compensate for) the PAC

Solation, gelation, and flocculation are processes involving colloids. The retardation of radionuclides may be reduced if they are associated with colloids and if the colloids are able to migrate through the rock pores and fractures. Flocculation of colloids containing radionuclides could produce larger particles which might migrate faster along larger less tortuous paths (e.g., Cathles, et al., 1974). On the other hand, flocculation could enhance retardation if the larger particles formed are too big to move efficiently through the rock.

Speciation including complexation and chelation can result in higher or lower radionuclide concentrations in groundwater and favorably or adversely affect the retardation of radionuclides. Other processes that could favorably or adversely affect radionuclide retardation are hydrolysis, diffusion and dehydration. Hydrolysis can be considered a speciation process. Diffusion can retard radionuclide migration, as for example, when radionuclides traveling in the relatively fast flow in fractures diffuse into the relatively stagnant fluid of the matrix. The reverse can also occur where radionuclides in a stagnant portion of a repository system can diffuse into a flowing portion thus, contributing to radionuclide mobility.

Volatilization can be applied to those radionuclides that can exist in the gas phase as well as the liquid phase. Examples are C-14, I-129, and Kr-85. In the unsaturated zone, these radionuclides can migrate to the accessible environment while either in the liquid or gas phase. Time spent in the gas phase will reduce the retardation when compared to mobility in the liquid phase.

It is likely that desorption and dissolution of radionuclides would enhance their mobility. These processes would tend to increase the concentrations of the radionuclides in the flowing groundwater. However, one can conceive of situations where mobility is reduced. For example, desorption of nonradioactive solutes can free up surfaces on which radionuclides can sorb.

Neither isotopic fractionation nor radioactive decay will significantly affect retardation. Isotopic fractionation is measured in parts per thousand for light stable isotopes. For the heavy radionuclides the effect is minimal. Alpha recoil is one type of fractionation that may be measurable, but its effect on transport is likely to be insignificant.

Anion exclusion is likely to contribute to reduction in radionuclide retardation. Evidence for this process has come from tests at the Cambric site on the Nevada Test Site where ruthenium in presumably an anionic state migrated much faster than expected from results of batch sorption tests (Coles and Ramspott, 1981).

Evaporation and condensation are processes involving the movement of water in the gas phase. These processes short circuit the transport of radionuclides in the liquid phase. Thus, it is unlikely that these processes will contribute to the reduction of retardation of radionuclides, except in the case where evaporation increases ionic strength significantly and concomitantly increases radionuclide complexation and colloid flocculation.

Osmosis is a process that involves movement of chemical constituents through a semipermeable phase. In the partially saturated zone of Yucca Mountain, one can conceive of osmosis occurring where the gas phase is permeable to water vapor but impermeable to nonvolatile constituents. Solutes, like dissolved nonvolatile radionuclides, will remain immobile. Thus, this process should not reduce radionuclide retardation, except indirectly.

Coprecipitation and filtration of radionuclides should only contribute to retardation. Filtration of nonradionuclides could plug flowpaths.

Oxidized radionuclide-bearing phases generally have higher solubilities than the reduced forms. Thus, oxidation can reduce retardation. Reduction, on the other hand, will not result in reduced radionuclide retardation.

Microbial processes can affect speciation which in turn can affect retardation. The metabolic processes of some microbes (e.g., GS-15) can reduce oxidized uranium in solution and precipitate a uraninite while oxidizing iron phases. Organic material coating surfaces can control the sorption of radionuclides.

The strength of the radiation field decreases quickly with distance from the emplaced waste. As a result, radiolysis and metamictization will probably not directly affect radionuclide retardation in the farfield. However, the production of radiolytic species in the nearfield when transported to the farfield can affect radionuclide mobility there. Corrosion is a process that is assumed to be applied to metallic material like waste canisters and not to farfield materials which may undergo the equivalent processes, alteration and dissolution. Thus, corrosion is considered in the portion of this PAC describing the engineered barrier system. However, corrosion of waste package components can indirectly adversely affect radionuclide migration in the farfield as well. For example, hydrolysis of corrosion products (Fe^{2+}, Cr^{3+}) can lead to acidic conditions locally causing increased solubility of some radionuclides. Competitive sorption of corrosion products may be another process reducing radionuclide retardation.

Ostwald ripening, if it occurs, results in the conversion of small crystals to larger crystals, thus reducing surface area. Conceivably, this could result in fewer sorption sites and less retardation. However, the extent of this process and that of devitrification may not be great enough to affect the performance of the repository over the period of regulatory concern.

Alteration of minerals along the flowpath can affect radionuclide mobility. For example, the zeolites are susceptible to alteration via ion exchange, which may reduce or increase the retardation of radionuclides depending upon the cations involved in the exchange. The zeolites may undergo alteration to other minerals which are less sorbing. Formation of clays from framework silicates, on the other hand, can increase the retardation of radionuclides.

If one assumes that magma will not intrude the repository nor will igneous activity occur in vicinity, the highest temperatures expected in the repository should be less than 250 °C, so melting of tuff minerals will not occur.

The catalysis of reactions reducing radionuclide retardation is uncertain. Rates of reactions play a key role in the performance of the geologic setting. Catalysis of some reactions can reduce radionuclide retardation while catalysis of other reactions can increase retardation. The DOE stated in the SCP that credit would not be taken for sorption in fractures due to the fast flow rates which preclude sorption reactions.

Expansion and contraction should have no effect on radionuclide retardation except in an indirect manner, whereby these processes affect flow conditions which influence retardation.

DOE has indicated that it will use a minimum Kd strategy to describe the effects of sorption on retardation at Yucca Mountain (Meijer, 1992). This strategy is based on batch sorption experiments involving crushed tuff and waters that simulate those expected in the repository. The parameters derived from these batch experiments will be compared to the results from a limited number of dynamic flow-though column experiments. If dynamic experiments indicate less retardation than would be calculated from the corresponding batch sorption test, the Kd will be adjusted to the lower value. This process will be carried out for all the tests, producing a minimum Kd for each radioactive element.

DOE will not be able to experimentally simulate every chemical and physical condition or process expected in the repository. In order to consider conditions and processes not simulated experimentally, DOE is planning to model those to determine their effects on radionuclide retardation. This modelling will invariably require certain assumptions. Some of these assumptions can be tested. Others cannot be tested and will thus constitute a technical uncertainty.

Degradation of rock strength

It is assumed that in this regulatory requirement topic, the phrase "geochemical processes that would degrade rock strength" applies only to the geologic setting outside of the engineered barrier system. "Geochemical processes that degrade rock strength" in the engineered barrier system are considered in the part of this regulatory requirement topic: "geochemical processes that would adversely affect performance of the engineered barrier system." The engineered barrier system is defined in the rule as the waste packages and the underground facility. The underground facility, in turn, is defined in the rule as the underground structure, including openings and backfill materials, but excluding shafts, boreholes, and their seals. Rock strength is important in situations where rocks can deform or fracture such as around large manmade openings or natural caves or caverns. In the geologic setting between the engineered barrier system and the accessible environment, these features are uncommon in the natural environment as suggested from existing drill hole data. Unless it can be demonstrated otherwise, through site characterization, it is assumed that large openings do not exist in the geologic setting. However, shafts, boreholes, and seals, which are excluded from the engineered barrier system, are places where rock strength could be important. If improperly designed, collapse of these features after permanent closure could produce fast pathways for radionuclide release. It is assumed, however, that the boreholes and shafts will be backfilled so as to minimize the effect of collapse. Thus, degradation (lessening) of rock strength, in the farfield would not lead to a potentially adverse condition. Consequently, it is assumed rock strength is important only near the repository openings of the engineered barrier system. Examples of geochemical processes that could affect rock strength are listed in Table 3.

Table 3. Geochemical Processes Potentially Degrading Rock Strength*

precipitation	U	diffusion	U	volatilization	U
dissolution	L	dehydration	L	nucleation	U
sorption	U	oxidation	U	anion exclusion	U
desorption	U	reduction	U	osmosis	U
speciation	U	hydrolysis	L	melting	U
solation	U	radiolysis	U	crystallization	U
gelation	U	microbial processes	L	coprecipitation	U
evaporation	U	radioactive decay	U	devitrification	£
condensation	U	isotopic fractionation	U	ion exchange	U
alteration	L	metamictization	L	Ostwald ripening	U
flocculation	U	catalysis	£	corrosion	U
expansion	L	contraction	L	filtration	U

*U = process is considered unlikely to contribute to PAC
L = process is considered likely to contribute to PAC
£ = process is considered likely to affect (i.e., contribute to or compensate for) the PAC

The table above lists the processes that are likely, unlikely and uncertain to contribute to the PAC. Thus, dissolution, alteration, dehydration, hydrolysis, metamictization, and expansion and contraction are likely to contribute to the PAC. It is uncertain what contribution catalysis and devitrification will have on the degradation of rock strength. All other processes from the table should not degrade rock strength. It is assumed that in the farfield very little metamictization (radiation damage) will occur. Likewise, as described for processes reducing radionuclide retardation, the amount of devitrification will be minimal over the lifetime of the repository.

Adverse effect on performance of the engineered barrier system:

The exact spatial limits of the engineered barrier system must be established so that appropriate geochemical processes can be considered. Included within the engineered barrier system are pillars between drifts and rock in drift walls out to the extent it has been grouted. As a result, the environment of the engineered barrier system can vary from an unperturbed natural setting to a fully engineered setting. The broad range of processes expected for these settings will reflect the variation in the settings. The use of the phrase "performance of the engineered barrier system" is interpreted to mean that the existence of this PAC will be evaluated based on performance levels required in 60.113(a)(1). These performance levels include substantially complete containment within the waste packages for a period not less than 300 years nor more than 1,000 years after permanent closure of the geologic repository and the release rate of any radionuclide from the EBS shall not exceed one part in 100,000 per year of the inventory present at 1,000 years following permanent closure. The phrase "adversely affect" is interpreted as a decrease in the containment capability of the waste packages and/or an increase in the radionuclide flux across the waste package and underground facility boundaries. At the Type 3 level, the processes listed as likely to contribute to the PAC need not adversely affect the performance of the EBS to the extent that the performance objective is not met. These processes need only decrease capabilities for substantially complete containment and increase radionuclide flux across the EBS/geologic setting boundary.

Table 4 lists the geochemical processes to be considered in evaluating which ones could adversely affect the EBS. In comparing this table with the one developed for geochemical processes that reduce radionuclide retardation it is apparent that additional processes are likely to contribute to this PAC. Processes like evaporation, condensation, and osmosis are included as likely. Evaporation can produce brines in contact with the waste canisters which can promote corrosion. Condensation and osmosis can increase the quantities of water in the vicinity of the EBS and enhance corrosion or radionuclide flux.

Filtration can plug flow paths and thus limit free drainage. Likewise, metamictization, or radiation damage, is expected in the EBS environment.

Detailed Safety Review Supported by Analyses (Type 4) Rationale:

The staff considers that there may be a high potential risk of noncompliance with the applicable regulatory requirements because, for the Yucca Mountain site, there are several Key Technical Uncertainties. These uncertainties could cause a high risk of noncompliance with both the overall system performance objective and subsystem performance objective concerns. Therefore, the staff considers that the findings made under this requirement may be highly uncertain because of the following Key Technical Uncertainties.

This concern of high risk of noncompliance will necessitate analysis above and beyond that required for a Type 3 safety review in order to assure that the uncertainties and potential effects on performance have been minimized to the extent practical.

Key Technical Uncertainty Topic: Uncertainty in identifying geochemical processes that reduce radionuclide "retardation."

Table 4. Geochemical Processes Potentially Adversely Affecting the Performance of the Engineered Barrier System*

precipitation	L	diffusion	L	volatilization	L
dissolution	L	dehydration	L	nucleation	£
sorption	L	oxidation	L	anion exclusion	L
desorption	L	reduction	L	osmosis	L
speciation	L	hydrolysis	L	melting	U
solation	L	radiolysis	L	crystallization	U
gelation	L	microbial processes	L	coprecipitation	L
evaporation	L	radioactive decay	L	devitrification	U
condensation	L	isotopic fractionation	U	ion exchange	£
alteration	L	metamictization	L	Ostwald ripening	U
flocculation	L	catalysis	L	corrosion	L
expansion	L	contraction	L	filtration	L

*U = process is considered unlikely to contribute to PAC
L = process is considered likely to contribute to PAC
£ = process is considered likely to affect (i.e., contribute to or compensate for) the PAC

Description of Uncertainty: The segregation of geochemical processes into those whose contribution to the existence of the PAC are likely, unlikely, or uncertain, can be used to assign the appropriate level of review. Those processes that are unlikely to contribute to the PAC are assumed to be unlikely to affect performance. Thus technical uncertainties with regard to those processes would not be "key."

Consequently, those processes would be constrained to a Type 3 review. Processes whose contribution to existence of the PAC is likely or uncertain may affect performance. The technical uncertainties associated with these processes would be "key" and require Type 4 or Type 5 review. Those processes that could affect performance but have no associated technical uncertainties will be considered a Type 3 review.

The geochemical processes whose contribution to the PAC is likely or uncertain are listed in Table 5.

Performance Objectives at Risk: 10 CFR 60.112

Explanation of Nature of Risk: Modeling radionuclide retardation will involve studying the effect of numerous processes and interactions between many chemical components under various conditions expected at Yucca Mountain. Failure to consider processes may make it difficult for DOE to demonstrate compliance with the overall system performance objective.

Description of Resolution Difficulty: Compliance with this regulatory requirement topic will require a quantitative evaluation of the effect of each of the processes on radionuclide retardation. These processes

Table 5. Geochemical Processes Potentially Reducing Radionuclide Retardation*

precipitation	£	diffusion	£	volatilization	L
dissolution	£	dehydration	£	sorption	£
oxidation	L	anion exclusion	L	desorption	£
speciation	£	hydrolysis	£	solation	L
gelation	L	microbial processes	L	ion exchange	£
corrosion	£	alteration	£	flocculation	L
catalysis	£				

*U = process is considered unlikely to contribute to PAC
L = process is considered likely to contribute to PAC
£ = process is considered likely to affect (i.e., contribute to or compensate for) the PAC

involve both radioactive and nonradioactive constituents of the repository and vicinity. The number of chemical components present at Yucca Mountain to be considered in this analysis will include key radionuclides and components introduced in the construction and characterization of the repository, corrosion products from the EBS, and components indigenous to the system. Geochemical modeling which will be used to demonstrate compliance with this regulatory requirement topic involves the simultaneous solution of linear and nonlinear equations representing mass balance and mass action respectively of the chemical components. The large number of components, processes, and conditions expected at the site precludes quantitative characterization of all possible (and expected) combinations of these parameters. Indications are that the DOE will use the minimum Kd approach to calculate radionuclide retardation (Meijer, 1992). This simplifying approach combines some experimental data with assumptions on water-rock interactions. As a result, some geochemical processes will not be characterized quantitatively and thus, remain uncertain.

The number of combinations of processes, components, and conditions is so great at Yucca Mountain as to make it unlikely that all will be considered in detail prior to submittal of a License Application. In order to minimize the number of possible combinations of processes, components, and conditions expected at Yucca Mountain, but not evaluated by DOE, the NRC staff and CNWRA personnel will need to continue geochemical modelling exercises in efforts such as iterative performance assessment and auxiliary analyses utilizing existing computer codes.

Key Technical Uncertainty Topic: Uncertainty in identifying geochemical processes that adversely affect the EBS.

Description of Uncertainty: The segregation of geochemical processes into those whose contribution to the existence of the PAC are likely, unlikely, or uncertain, can be used to assign the appropriate level of review. Those processes that are unlikely to contribute to the PAC are assumed to be unlikely to affect performance. Thus technical uncertainties with regard to those processes would not be "key." Consequently, those processes would be constrained to a Type 3 review. Processes whose contribution to existence of the PAC is likely or uncertain may affect performance. The technical uncertainties associated with these processes would be "key" and require Type 4 or Type 5 review. Those processes that could affect performance but have no associated technical uncertainties will be considered a Type 3 review.

The geochemical processes whose contribution to the PAC is likely or uncertain are listed in the Table 6.

Table 6. Geochemical Processes Potentially Adversely Affecting the Performance of the Engineered Barrier System*

precipitation	L	diffusion	L	volatilization	L
dissolution	L	dehydration	L	nucleation	£
oxidation	L	anion exclusion	L	desorption	L
reduction	L	osmosis	L	speciation	L
hydrolysis	L	solation	L	radiolysis	L
crystallization	L	gelation	L	microbial processes	L
coprecipitation	L	evaporation	L	radioactive decay	L
condensation	L	ion exchange	£	alteration	L
metamictization	L	flocculation	L	catalysis	L
corrosion	L	expansion	L	contraction	L
filtration	L				

*U = process is considered unlikely to contribute to PAC
L = process is considered likely to contribute to PAC
£ = process is considered likely to affect (i.e., contribute to or compensate for) the PAC

Performance Objectives at Risk: 10 CFR 60.113(a)(1)

Explanation of Nature of Risk: Modeling of geochemical processes that may affect the performance of the EBS will include consideration of numerous combinations of processes, components, and conditions. Failure to consider all processes may make it difficult for DOE to demonstrate compliance with the subsystem performance objectives set forth in 10 CFR 60.113 (a)(1).

Description of Resolution Difficulty: Compliance demonstration of this regulatory requirement topic will require a quantitative evaluation of the effect of each of the processes on the performance of the EBS. These processes involve both radioactive and nonradioactive constituents of the repository, both manmade (or introduced) and indigenous. The range of conditions to be considered in demonstrating compliance with this PAC are more extensive than with the PAC on radionuclide retardation. Temperatures can vary up to 250 °C, groundwaters could be as dilute as rainwater or as concentrated as brine. Geochemical modeling which will be used to demonstrate compliance with this regulatory requirement involves the simultaneous solution of linear and nonlinear equations representing mass balance and mass action respectively of the chemical components. The large number of components, processes, and conditions expected at the site precludes quantitative characterization of all possible (and expected) combinations of these parameters.

The number of combinations of processes, components, and conditions is so great at Yucca Mountain as to make it unlikely that all will be considered in detail prior to submittal of a License Application. Some of the processes that are to be considered in demonstrating compliance with this regulatory requirement may include chemical and isotopic species that are not traditionally considered in geochemical modeling. This would require modification of existing codes and databases.

Detailed Safety Review Supported by Independent Tests, Analyses, or Other Investigations (Type 5) Rationale:

The staff considers that there may be the highest potential risk of noncompliance with this regulatory requirement topic because, for the Yucca Mountain site, the following Key Technical Uncertainties are the most difficult to resolve. Therefore, there might be a high residual risk of noncompliance with the performance objectives specified below because very little can be done to reduce the risk, or compensate for the risk using, for example, favorable site conditions or engineered features.

The potential for high residual risk of noncompliance in light of these Key Technical Uncertainties is sufficient that a detailed safety review supported by independent tests, analyses, or other investigations is justified.

Key Technical Uncertainty Topic: Uncertainty in determining the magnitude of the effect of the geochemical processes that reduce radionuclide "retardation."

Description of Uncertainty: The geochemical processes whose contribution to the PAC is likely or uncertain are listed in the Table 7.

Table 7. Geochemical Processes Potentially Reducing Radionuclide Retardation*

precipitation	£	diffusion	£	volatilization	L
dissolution	£	dehydration	£	sorption	£
oxidation	L	anion exclusion	L	desorption	£
speciation	£	hydrolysis	£	solation	L
gelation	L	microbial processes	L	ion exchange	£
corrosion	£	alteration	£	flocculation	L
catalysis	£				

*U = process is considered unlikely to contribute to PAC
L = process is considered likely to contribute to PAC
£ = process is considered likely to affect (i.e., contribute to or compensate for) the PAC

The degree to which each of these processes can reduce radionuclide retardation depends on many factors. These factors include thermodynamic properties for solids and aqueous and gaseous species such as Gibbs free energy of formation from the elements, enthalpy of formation from the elements, and entropy. Also concentrations of chemical components, activity coefficients, rate constants, and conditions like temperature and pressure, and flow rates are required. As a further illustration of the large number of parameters necessary for characterizing processes, one need only consider the triple layer model for surface complexation (sorption) where seven adjustable parameters are required (Turner, 1991).

Performance assessment calculations typically use a single retardation factor (R_f) to represent the attenuation of radionuclide transport. This factor is frequently based on an experimentally measured sorption coefficient (K_d), which is assumed to represent equilibrium sorption/desorption processes alone. However, other processes may contribute to retardation, including diffusion, dispersion, and precipitation. Although using R_f simplifies transport calculations, it is empirical in nature and has no theoretical basis for extrapolation beyond the particular conditions of the initial experiments. It is well-known that sorption of radionuclides on rock and mineral substrates are influenced by the physical and chemical characteristics of the groundwater (e.g., pH, composition, temperature) and of the substrate (e.g., mineralogy, surface area, surface properties). R_f (K_d) tends to be assigned as a "property" of the medium. This does not accurately reflect the role of systematic chemical variations in determining the extent of retardation of radionuclide migration. The use of R_f also does not allow discrimination between the contributions of various processes involved in retardation. Therefore, it is not clear how quantitative representation of retardation processes can be done using the R_f approach.

<u>Performance Objectives at Risk</u>: 10 CFR 60.112

<u>Explanation of Nature of Risk</u>: Uncertainty with regard to the numerical value of the parameters used in modeling the effects of the various geochemical processes on radionuclide retardation can make uncertain the demonstration of compliance with this regulatory requirement. Since all combinations of site-specific materials cannot be tested, demonstration of compliance will be uncertain. This uncertainty would make it harder to demonstrate compliance with the overall system performance objective.

<u>Description of Resolution Difficulty</u>: There are many physical and chemical parameters that affect retardation processes, many of which have synergistic effects. The use of simple representations of sorption and retardation, such as K_d and R_f, are uncertain when extrapolated to conditions other than those of the initial experiment. More robust models, such as surface-complexation models, require more parameters and additional types of experimental data. The latter represents state-of-the-art modelling, but model parameters are available for only a few radionuclides and a few sorbents. Surface-complexation approaches are also not currently applied to modeling transport of particulates and colloids.

The number of combinations of processes, components, rates and conditions is so great at Yucca Mountain as to make it unlikely that all will be considered quantitatively prior to submittal of the License Application. Some of the processes that are to be considered in demonstrating compliance with this regulatory requirement may include chemical and isotopic species that are not traditionally considered in geochemical modeling. This would require modification of existing codes and databases by NRC staff and CNWRA personnel and possible collection of experimentally determined thermodynamic and kinetic parameters by CNWRA personnel. The complexity of the interactions of the factors listed above make it difficult to reduce the uncertainties involved.

Key Technical Uncertainty Topic: Uncertainty in determining the magnitude of the effect of the geochemical processes that adversely affect the EBS.

Description of Uncertainty: The geochemical processes whose contribution to the PAC is likely or uncertain are listed in Table 8.

Table 8. Geochemical Processes Potentially Adversely Affecting the Performance of the Engineered Barrier System*

precipitation	L	diffusion	L	volatilization	L
dissolution	L	dehydration	L	nucleation	£
oxidation	L	anion exclusion	L	desorption	L
reduction	L	osmosis	L	speciation	L
hydrolysis	L	solation	L	radiolysis	L
crystallization	L	gelation	L	microbial processes	L
coprecipitation	L	evaporation	L	radioactive decay	L
condensation	L	ion exchange	£	alteration	L
metamictization	L	flocculation	L	catalysis	L
corrosion	L	expansion	L	contraction	L
filtration	L				

*U = process is considered unlikely to contribute to PAC
L = process is considered likely to contribute to PAC
£ = process is considered likely to affect (i.e., contribute to or compensate for) the PAC

These processes involve both radioactive and nonradioactive constituents of the repository, both manmade (or introduced) and indigenous. The range of conditions to be considered in demonstrating compliance with this PAC are more extensive than with the PAC on radionuclide retardation. Temperatures can vary up to 250 °C, groundwaters could be as dilute as rainwater or as concentrated as brine. Geochemical modeling which will be used to demonstrate compliance with this regulatory requirement involves the simultaneous solution of linear and nonlinear equations representing mass balance and mass action respectively of the chemical components. The large number of components, processes, and conditions expected at the site precludes quantitative characterization of all possible (and expected) combinations of these parameters.

The degree to which each of these processes can adversely affect the performance of the EBS depends on many factors. These factors include thermodynamic properties for solids and aqueous and gaseous species such as Gibbs free energy of formation from the elements, enthalpy of formation from the elements, and entropy. Also, concentrations of chemical components, activity coefficients, rate constants, and conditions like temperature and pressure, and flow rates are required.

Performance Objectives at Risk: 10 CFR 60.113(a)(1)

Explanation of Nature of Risk: Modeling of geochemical processes that may affect the performance of the EBS will include consideration of numerous combinations of processes, components, and conditions.

Failure to establish accurate values for the parameters associated with these processes may make it difficult for DOE to demonstrate compliance with this PAC. This failure would make it harder to demonstrate compliance with the overall system performance objectives.

Description of Resolution Difficulty: Compliance demonstration of this regulatory requirement topic will require a quantitative evaluation of the effect of each of the processes on the performance of the EBS. The number of combinations of processes, components, rates, and conditions is so great at Yucca Mountain as to make it unlikely that all can be fully considered prior to submittal of a License Application. Some of the processes that are to be considered in demonstrating compliance with this regulatory requirement may involve chemical and isotopic species that are not traditionally considered in geochemical modeling. As a result, thermodynamic and kinetic data do not exist for those species and would have to be determined experimentally or approximated. The complexity of the interactions of the factors listed above make it difficult to reduce the uncertainties involved.

Summary: The following assumptions have been made in assigning a Type 5 level of review to this CDS:

(1) All probable combinations of geochemical processes and associated conditions that potentially can reduce radionuclide retardation, or adversely affect the performance of the engineered barrier system can not be fully evaluated because of the intrinsic complexity of the interactions involved.

(2) Quantitative determination of all the thermodynamic and kinetic parameters necessary to characterize these processes can not be fully accomplished because of the intrinsic complexity of the interactions involved.

REVIEW STRATEGY:

Acceptance Review:

In conducting the acceptance review of information regarding geochemical processes which would reduce retardation of radionuclides, result in degradation of rock strength, or adversely affect the performance of the engineered system, the reviewer should determine if the information present in the license application and its references for determining compliance with the applicable regulatory requirement(s) (or the FCRG) is complete in technical breadth and depth as identified in the FCRG. The reviewer should determine whether all appropriate information necessary for the staff to review the information regarding geochemical processes which would reduce retardation of radionuclides, result in degradation of rock strength, or adversely affect the performance of the engineered system is presented such that the assessments required by the regulatory requirement(s) associated with total system and subsystem performance objectives or other technical criteria can be performed.

The information contained in the license application should be presented in such a way that the assumptions, data, and logic lead to a clear demonstration of compliance with the requirements. The reviewer should not be required to conduct extensive analyses or literature searches. The reviewer should also determine whether an appropriate range of alternative interpretations and models has been described.

Finally, the reviewer should determine if the U.S. Department of Energy (DOE) has either resolved all the NRC staff objections that apply to this requirement or provided all the information requested in Section 1.6.2 of the FCRG, for unresolved objections. The reviewer should evaluate the effects of any unresolved objections, both individually and in combinations with others, on: (1) the reviewer's ability to conduct a meaningful and timely review; and (2) the Commission's ability to make a decision regarding construction authorization within the three-year statutory period.

Safety Review:

This regulatory requirement topic is limited to consideration of geochemical processes which would reduce retardation of radionuclides, result in degradation of rock strength, or adversely affect the performance of the engineered system. It does not address geochemical conditions, although conditions and processes are intimately associated. Thus, this regulatory requirement topic does not consider geochemical conditions that could be potentially adverse. Geochemical conditions such as that described in the PAC concerning groundwater conditions in the host rock that might affect the engineered barrier system will be covered in Section 3.2.3.4 "Groundwater Conditions and the Engineered Barrier System" of the License Application. Likewise, other geochemical conditions such as groundwater conditions in the host rock that are not reducing will be addressed in Section 3.2.3.6 "Groundwater Conditions in the Host Rock That are not Reducing" of the License Application.

Following the Acceptance Review, the first step will be to evaluate DOE's analyses to determine if the following basic assumptions are correct:

(1) All probable combinations of geochemical processes and associated conditions that potentially can reduce radionuclide retardation, or adversely affect the performance of the engineered barrier system can not be fully evaluated because of the intrinsic complexity of the interactions involved.

(2) Quantitative determination of all of the thermodynamic and kinetic parameters necessary to characterize all probable combinations of geochemical processes can not be fully accomplished because of the intrinsic complexity of the interactions involved.

If the above assumptions are met, the staff will follow the review strategy described here. If these assumptions are not met, the staff review may require a different review strategy for evaluating DOE's demonstration of compliance with the applicable regulatory requirements. It is expected, however, that any deviation from this assumption will be known well in advance of the time a license application is submitted, and this strategy shall be revised in accordance with such new information as it becomes available to the staff.

In conducting the Safety Review, the reviewer will, at a minimum, determine the adequacy of data and analyses presented in the license application to support the DOE's demonstrations regarding 10 CFR 60.122(c)(8). Specifically, DOE will need to: (1) provide information to determine the degree to which the PAC is present, but undetected; (2) provide information that demonstrates to what degree the PAC is present: (3) assure the sufficiency of the lateral and vertical extent of the data collection; and (4) evaluate the information presented under items (1) and (2) above, with assumptions and analysis methods that adequately describe the presence of the PAC and ranges of relevant parameters. The specific aspects of the license application on which the reviewer will focus are discussed below, and the Acceptance Criteria will be identified in Section 3.0 of this Review Plan.

In conducting the Safety Review, the staff should confirm that DOE has submitted the following: (1) information regarding geochemical processes which would reduce retardation of radionuclides, (2) information regarding geochemical processes which would result in degradation of rock strength, and (3) information regarding geochemical processes which would adversely affect the performance of the engineered barrier system. This information is expected to include adequate data concerning mineralogy, geochemistry, hydrology, and structural geology to allow assessment of relevant geochemical processes. This information is also expected to include adequate data concerning the engineered systems to allow assessment of the interaction of geochemical processes with the engineered barrier system.

DOE will also need to explain how models are supported that are used to assess the presence or absence of the PAC. Analyses and models that will be used to predict future conditions and changes in the geologic setting shall be supported by an appropriate combination of methods such as field tests, laboratory tests that are representative of field conditions, monitoring data, and natural analog studies. For purposes of determining the presence or absence of the PAC, investigations should extend from the ground surface to a depth sufficient to determine critical pathways for radionuclide migration from the underground facility. Investigations should be sufficient to demonstrate a suitable understanding of potential effects of geochemical processes on radionuclide retardation, rock strength, or performance of the engineered barrier system such that reasonable bounds can be placed on the different conceptual models.

In conducting the aforementioned evaluations, the reviewer should determine that DOE uses: (1) analyses that are sensitive to evidence of the PAC; and (2) assumptions that are not likely to underestimate its effects. In general, the reviewer will assess the adequacy of DOE's investigations regarding the likelihood of this PAC, both within the controlled area and outside the controlled area, as necessary, in the manner defined in 10 CFR 60.21(c)(1)(ii)(B).

Reviewers will rely on staff expertise and independently acquired knowledge, information, and data such as the results of research activities being conducted by the NRC's Office of Nuclear Regulatory Research, in addition to that provided by the DOE in its license application. The reviewer should focus on additional data which can refine knowledge of information regarding geochemical processes which would reduce retardation of radionuclides, result in degradation of rock strength, or adversely affect the performance of the engineered barrier system, and should perform, as necessary, additional analyses to confirm the resolution capabilities of the methodologies. The reviewer must have access to a body of knowledge regarding these and other critical considerations in anticipation of conducting the review to assure that DOE investigations to resolve the presence or absence of geochemical processes which would reduce retardation of radionuclides, result in degradation of rock strength, or adversely affect the performance of the engineered system, are sufficient in scope and depth to provide the information to resolve the concerns. For example, research undertaken in the CNWRA Geochemistry, Sorption, Engineered Barrier System, and Geochemical Natural Analogs research projects are expected to provide data relevant to the assessment of information regarding geochemical processes which would reduce retardation of radionuclides, result in degradation of rock strength, or adversely affect the performance of the engineered system.

Finally, investigations in the following DOE site characterization program study plans are expected to produce data and analyses needed to help in the review described above to address the presence or absence of this PAC:

STUDY PLAN NO.	TITLES
8.3.1.2.2.7	Hydrochemical Characterization of the Unsaturated Zone (DOE, 1990a)
8.3.1.2.3.2	Characterization of the Yucca Mountain Saturated-Zone Hydrochemistry (DOE, 1992d)
8.3.1.3.2.1	Mineralogy, Petrology, and Chemistry of Transport Pathways

8.3.1.3.2.2	History of Mineralogic and Geochemical Alteration of Yucca Mountain (DOE, 1992b)
8.3.1.3.3.4	Conceptual Model of Mineral Evolution (in preparation)
8.3.1.5.1.4	Analysis of the Paleoenvironmental History of the Yucca Mountain Region (DOE, 1991e)
8.3.1.5.1.5	Paleoclimate-Paleoenvironmental Synthesis (in preparation)
8.3.1.5.2.1	Characterization of the Quaternary Regional Hydrology (DOE, 1992g)

Reports presenting the results from additional study plans related to this PAC, when available, should also be reviewed.

Detailed Safety Review Supported by Analysis:

A Detailed Safety Review will be needed to evaluate the Key Technical Uncertainties regarding identification of processes that contribute to the PAC and magnitude of effects of geochemical processes on radionuclide retardation and performance of the EBS. This will ensure that DOE has adequately demonstrated Items (1)-(4), listed in the previous section (See Section 2.2.1 (Safety Review), 3rd paragraph). Activities performed in this Detailed Safety Review will help to assure that DOE has adequately addressed and resolved the Key Technical Uncertainties so that they do not lead to noncompliance with 10 CFR 60.112, and 10 CFR 60.113(a)(1).

For the Key Technical Uncertainty regarding identification of processes that contribute to the PAC, examples of specific review activities that will be required include: (1) review and analysis of processes anticipated at the site; (2) evaluation of uncertainties in the reported analytical data; and (3) determination of the potential implications of the reported anticipated processes on radionuclide retardation, and effects on the performance of the EBS. This review will require familiarity with analytical chemistry and error propagation methods. The use of equilibrium geochemical codes such as EQ3 will be used to evaluate the analytical data on groundwater chemistry. To help determine the potential implications of the reported groundwater chemistry to inhibition of radionuclide transport, other codes such as MINTEQA2 (Allison et al., 1991) may be used. It may also be appropriate to assess the quality and traceability of data and information by utilizing staff with expertise in review of quality assurance programs.

For the Key Technical Uncertainty specifically applied to processes concerning retardation of radionuclides, examples of specific review activities that will be required include: (1) review and analysis of models used to represent retardation processes in radionuclide transport calculations, including the assumptions and uncertainties associated with the models; and (2) evaluation of the experimental, field, and natural analog data that were used to validate the models and to demonstrate their capability to predict radionuclide retardation and transport under varying geochemical conditions. The NRC staff will need to model radionuclide retardation and transport using codes and models developed by DOE or by CNWRA for the NRC. Published experimental, field, and natural analog data, including those generated for NRC by CNWRA, will be used to develop, validate, and test the predictive capabilities of the models. Sensitivity analyses will need to be performed to evaluate the statistical reasonableness of model parameters. For key technical uncertainties it may also be appropriate to assess the quality and traceability of data and information by also using staff with expertise in review of quality assurance programs.

For the Key Technical Uncertainty specifically applied to processes adversely affecting the performance of the engineered barrier system, examples of specific review activities that will be required include: (1) review and analysis of models used to represent processes affecting EBS performance, including the assumptions and uncertainties associated with the models; and (2) evaluation of the experimental, field, and natural analog data that were used to validate the models and to demonstrate their capability to predict EBS performance under varying geochemical conditions. Given the special materials and conditions that are anticipated in the EBS, existing codes will have to be modified to test these special situations and sensitivity analysis performed to ascertain which parameters are important to the performance of the EBS.

Detailed Safety Review Supported by Independent Tests, Analyses or Other Investigations:

A Detailed Safety Review, independent modeling, and use of the results of staff investigations, will be needed for the Key Technical Uncertainties concerning the magnitude of the effect of geochemical processes that reduce retardation of radionuclides, or adversely affect the performance of the engineered system. This will ensure that DOE has adequately demonstrated Items (1)-(4) listed in the section on Safety Review (see section 2.2.1, para. 4).

For Key Technical Uncertainties regarding the magnitude of effects of geochemical processes on radionuclide retardation and performance of the EBS, the staff's Detailed Safety Review will be supported by uncertainty analysis to identify processes and combinations of processes most likely to contribute to the PAC. Independent calculations using computer codes such as EQ3 and MINTEQA2 will be conducted by NRC staff to evaluate the analytical data reported by DOE and to determine the implications of the measured groundwater compositions to radionuclide retardation and transport. In order to have better confidence in the data presented by DOE, independent determinations of groundwater compositions for the partially-saturated hydrologic zone of Yucca Mountain may be performed by NRC staff using methods which may or may not be the same as that used by DOE. It may also be appropriate to assess the quality and traceability of data and information by utilizing staff with expertise in review of quality assurance programs.

For the Key Technical Uncertainty as applied to radionuclide retardation processes evaluations will be supported by the results of staff investigations that may include experiments to study radionuclide sorption and retardation processes, and coupled geochemical-hydrologic modeling work. It is anticipated that these experiments and modeling activities will help identify the key parameters that control radionuclide retardation and transport, and help determine scientifically defensible approaches to coupling geochemistry and hydrology for performance assessment calculations. It may also be appropriate to assess the quality and traceability of data and information by utilizing staff with expertise in review of quality assurance programs.

For the Key Technical Uncertainty as applied to processes that adversely affect the performance of the engineered barrier system, evaluations will be supported by the results of staff investigations that may include experiments to study the effects of various geochemical processes on the effectiveness of the engineered barrier system to isolate waste. Since unique materials and conditions may be anticipated in the engineered barrier system, independent quantitative analysis of selected processes of selected processes that can affect the performance of the EBS will be required to evaluate the DOE demonstration of compliance with the regulatory requirement. Currently available codes would have to be modified and sensitivity analysis performed to determine the effect of various parameters on the performance of the EBS.

RATIONALE FOR REVIEW STRATEGY:

In view of the complexity of the key technical uncertainties addressed above, it is appropriate that the NRC conduct the independent activities described in order to (1) develop the licensing tools and technical basis necessary to judge the adequacy of DOE's license application, (2) assure sufficient independent understanding of the basic physical processes taking place at the geologic repository, and (3) maintain an independent but limited confirmatory research capability under NRC auspices.

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Date of Analysis:	August 3, 1993

APPLICABLE REGULATORY REQUIREMENTS FOR EACH TYPE OF REVIEW:

Type 1:

10 CFR 60.122(c)(8)
10 CFR 60.21(c)(1)(ii)(B)
10 CFR 60.21(c)(1)(ii)(F)

Type 3:

10 CFR 60.122(c)(8)

Type 4:

10 CFR 60.122(c)(8)

Type 5:

10 CFR 60.122(c)(8)

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