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Construction of Scenarios for Nuclear Criticality at the Potential Repository at Yucca Mountain, Nevada

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Civilian Radioactive Waste Management System

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ABSTRACT

The fissile material contained in the radioactive waste emplaced at the potential Yucca Mountain repository has the potential to undergo nuclear criticality under certain conditions. The features, events, and processes that could lead to critical configurations are discussed in this report. Several potential critical configurations have been identified for inclusion as TSPA-VA sensitivity studies. This report does not discuss the PA consequences of critical configurations – only their potential for occurring.

Although waste-package design and fissile-material loading requirements preclude criticality in intact containers, as waste packages fail and subsequently admit water, potential critical configurations have been postulated at three locations. These are primarily inside waste packages and, to a much lesser extent, in the near field (in the repository drift) and in the far field (in the unsaturated and saturated zones). The conditions leading to in-package criticality primarily require the presence of water to act as a neutron moderator; depending on the waste form, some degree of mechanical collapse or chemical degradation must also occur. Potential critical configurations involving commercial spent nuclear fuel (SNF), DOE SNF and plutonium in glass or ceramic are suggested for inclusion in TSPA-VA.

Most near-field and far-field critical configurations require mechanisms to re-concentrate the fissile material after it has been transported from the waste packages. No credible geochemical or transport processes have been identified that will readily do this in times less than those required for ore-body formation. One near-field critical configuration to be analyzed in TSPA-VA involves extensive failure of the bottom of a waste package resulting in the waste being "dumped" into a pool of water in the drift. Formation of far-field critical configurations appear even less credible. The re-concentration processes are essentially those of epigenetic ore-body formation and require the presence of reducing agents (such as organic materials). Although organic deposits are not thought to be present at Yucca Mountain, this potential critical configuration will be included in the TSPA-VA analyses to provide an example of the PA impacts of far-field criticality.

This report includes a large-size complete FEP diagram as an attachment.

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Richard van Konynenburg, Henry Loo, John Massari, and Mark Nutt all made valuable contributions during the review of the initial version of the FEP diagram. Their comments resulted in the FEP diagram more closely reflecting the neutronic processes thought to occur in the waste package.

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John Massari provided much pertinent information about waste-package and waste-form degradation processes potentially leading to criticality.

Mary Heerdt skillfully produced the FEP diagrams and formatted the document, and Isaac Block did much of the graphics.

Reviews were completed by Jack Gauthier and Jerry McNeish.

1.0 INTRODUCTION

Scenarios for potential post-closure nuclear criticality have been developed based on the Abstraction/Testing workshop on criticality held on March 18–20, 1997 (CRWMS M&O, 1997c). At that workshop, experts in nuclear physics and nuclear engineering met with geotechnical experts to identify the areas most of concern for criticality. The workshop identified three physical regions where criticality events should be considered: (1) inside the waste package, (2) in the near field immediately surrounding the waste package (considered for these analyses to be the emplacement drift only), and (3) in the far field (defined as the host rock surrounding the emplacement drift).

This report presents an introduction to the nuclear and geotechnical issues related to criticality, an introduction to scenario analysis, and a discussion of features, events, and processes (FEPs) that define conditions under which a criticality event might occur. A logically connected sequence of FEPs defines a scenario; each criticality scenario has an initiating FEP, and concludes with the formation of a potentially critical configuration and the associated PA consequences. No attempt has been made here to screen scenarios to identify those that are improbable (either physically or probabilistically), or of low consequence. Such screening must be done by expert reviewers, who will provide physical or probabilistic justifications for either retaining or dismissing any of the scenarios presented here.

Considerable criticality-analysis work has also been done by the Waste-Package Design organization of the Yucca Mountain Project CRWMS M&O Contractor. Many of the potential critical configurations identified here have been analyzed already (as documented later in this report); in some cases, their analyses have shown that scenarios in this FEP diagram are unimportant to potential post-closure criticality. For the sake of completeness and to show explicitly the arguments making them unimportant, some of these scenarios are retained in the tree; future analyses may disregard them. The first such document has been completed with inputs from both Performance Assessment and Waste-Package Development (CRWMS M&O, 1997d).

1.1 Neutronics

A fission event occurs when a neutron interacts with a fissile nucleus, causing the nucleus to split (fission) and release energy. The fission process produces several energetic neutrons per fission event. As neutrons pass through other materials (such as water, air, rock, etc.), they can be absorbed, or slowed down by scattering. A configuration of nuclear fuel and other materials is said to be critical if the fission process is self-sustaining; i.e., the number of neutrons produced is equal to the number lost by absorption or leakage. The ratio of neutron-population changes from generation to generation in a fissioning system is the *neutron multiplication factor*, k. In a theoretical system of infinite size, the multiplication factor is k_{∞}. For a finite system, where there is leakage of neutrons away from the fissile material, the measure used is the effective multiplication factor, k_{eff}. Neutrons produced by fissions have an energy range of approximately 1 to 10 million electron volts (MeV), with an average of approximately 2 MeV; these are called "fast" neutrons. As neutrons scatter from other materials, they can slow down to kinetic energies in the range of a few eV or less. The latter are called thermal neutrons; neutrons in the energy range above thermal to a few keV are called epithermal. Some nuclides can fission only when interacting with fast neutrons (e.g., ^{238}U and ^{232}Th), but others can fission with neutrons of any energy (e.g., ^{235}U, ^{239}Pu, and other nuclides). The term *fissile* nuclides is applied to those that can fission with neutrons of any energy; *fissionable* nuclides require fast neutrons. It is not expected that fissionable nuclides will make an important contribution to the criticality considerations at Yucca Mountain, because of the small cross section for fast neutrons.

The measure of interactions (e.g., scattering, fission, or absorption) between moving particles (neutrons) and other nuclei is called the cross section. Elastic-scattering cross sections for neutrons are greater for the lighter nuclei (hydrogen, oxygen, silicon, etc.). It is by elastic or inelastic scattering that fast neutrons slow to thermal energies, a process called *moderation*. The fission cross sections for fissile nuclei are larger for the absorption of thermal neutrons than for fast neutrons. Therefore the mixing of a moderator with fissile material enhances fission reactions by increasing the fraction of neutrons at thermal energies, where fissions are much more likely. A greater amount of kinetic energy is lost per collision when the scattering nuclei are very light than when the scattering nuclei are heavier. Water, which contains light hydrogen nuclei is a much more efficient moderator than the tuff rock found at Yucca Mountain, which is composed primarily of SiO_2, because it requires many more collisions to thermalize fission neutrons in SiO_2 than in water. Because it increases the probability of fissions, an efficient moderator like water reduces the mass of fissile material necessary to achieve criticality. In a mixture of tuff and water, moderation is not as efficient as in water and any criticality event would require a larger fissile mass and would most likely occur with higher-energy (epithermal) neutrons.

TALK ABOUT ABSORPTION

REASON YOU WANT EFFICIENT MODERATOR IS TO REDUCE PROB OF LEAKAGE & ABS.

Nuclear criticality potentially can occur in a post-closure repository environment provided several conditions are met: primarily, there must be a sufficient mass of fissile material present, and there must be sufficient moderator to thermalize (or near-thermalize) the neutron spectrum. Water is the best common moderator found in a geologic environment, although other materials, such as SiO_2 in glass or tuff rocks can also act as moderators. Other factors, such as neutron absorbers ("poisons") and scatterers (reflectors) change the amounts of fissile materials and moderators needed to form a potentially critical configuration.

1.2 Geologic Processes

Repository waste packages are designed and will be engineered to prevent criticality events from occurring while the packages are intact. Even if a package were to fill with water, there is a sufficient quantity of neutron-absorbing material provided to prevent criticality in an as-designed and engineered waste package.

It is expected that in a repository environment of elevated temperatures with the presence of water (liquid and/or vapor) and other hostile environmental agents, the waste packages will eventually degrade to the point where water vapor and oxygen can come in contact with the waste. The rates and modes of waste-package corrosion depend on temperature, on oxygen content in the water and the repository drifts, and on chemical characteristics of the water present in the drifts (water-contact modes), AS ~~are~~ discussed below. Initial failure of the waste packages is expected to be in the form of small perforations (shown as "penetration" in the FEP diagrams). More extensive degradation, to the point where there are large enough holes that there is no flow restriction into and out of the package, and possibly loss of mechanical integrity, is specified as "breach" in the FEP diagrams.

The environment inside a failed waste package is expected to contribute to degradation of the waste form through oxidation and attack by aggressive products of radiolysis of the air and water, and reaction with waste-package materials. These processes can release fissile materials from the waste form and make them available to be transported elsewhere (possibly separately from the criticality-control neutron absorbers). Fissile materials and other contaminants can be mobilized in groundwater either as solutes or as colloidal suspensions (for short distances, larger particles can also be moved by geologic forces). Colloids can include both intrinsic colloids (composed of the waste-form material), and pseudo-colloids, composed of fissile material adsorbed onto other colloids (such as hydrous ferric oxide particles). Depending on the timing of release, the fissile-material inventory available to be transported can differ due to radioactive decay. For example, if waste-form mobilization occurs in less than about 24,100 years, less than half of the ^{239}Pu will have decayed to ^{235}U, and many other factors affecting criticality will be different.

Eventually, the waste-package breach will permit any available water seepage in the drift to enter the waste package and to transport fissile material from the package to the repository drift. Concentrations of fissile material can range from less than 10^{-6} g/l for some solutes to $\sim 10^{3}$ g/l for some colloidal suspensions (Wanner and Forest, 1992; Nitsche et al., 1993). Uranium solubility experiments have shown it to have a relatively large solubility in groundwater, compared with plutonium. Neutron absorbers can range from the very soluble borates to the relatively insoluble rare-earth element fission products (M&O, 1997g). It is generally necessary for the neutron absorbers to be separated from the fissile material, and for the fissile material to become concentrated, before a criticality can occur. Significant separation of absorbers from fissile material can occur because of differences in waste-form alteration rates, solubilities, sorption, and filtration. Concentrations of fissile materials high enough for criticality exist within the waste package; re-concentration of mobilized fissile materials can be envisioned to occur immediately outside the waste package and in the host rock from precipitation of solutes, or filtration of colloids. Mechanisms for precipitation include change in oxidation state; filtration can be either geochemical or mechanical.

The materials immediately surrounding the waste package may provide an environment suitable for re-concentration of fissile material and formation of a critical configuration. Present are concrete, iron, water, and many corrosion products.

Groundwater passing through repository materials may create a "carrier plume" — water with a significantly altered pH and mineral content (compared with ambient groundwater, such as that from well J-13). The geochemical behavior of fissile materials in the carrier plume may be considerably different from that in unaltered groundwater. In the far field, repository thermal effects, combined with geochemical alterations from the carrier plume, may provide locations where critical configurations can form. For example, stratigraphic layers beneath the repository in the unsaturated zone may become altered, such that they can concentrate fissile materials either by sorption of solutes, or trapping or filtration of colloids.

Concentration mechanisms must be weighed against the otherwise generally dispersive behavior of groundwater-transport processes. Contaminants are transported in the unsaturated and saturated zones by diffusion and groundwater advective flow. Unsaturated flow can occur in both the rock matrix and in fractures, with greatly different velocities and mass fluxes. The various geohydrologic rock units have different flow characteristics and different amounts of fracturing. In the saturated zone, the strata may confine water flow to limited volumetric regions.

1.3 Basic Organization and Use of FEP Trees for Scenario Analysis

Numerous features, events, and processes thought to be important to the function of a repository have been suggested by principal investigators (PIs) in this and other repository programs (e.g., those in Sweden, Switzerland, the UK, etc.). In order to establish how individual FEPs contribute to repository overall behavior they need to be put into some context describing the contributions of those FEPs and their relation to other FEPs. The method of establishing that context is a generalized event tree. The criticality event tree consists of a series of FEPs organized in a number of vertical branches. Each branch is composed of a generally time-ordered sequence of FEPs that are intended to reasonably describe contact of water with waste containers (of any type), the subsequent corrosion of the container and its contents, the mobilization of the degradation products, and the possible accumulation of the fissile material into a potentially critical configuration. A "scenario" is defined here to be a single, simply connected path from the top of the tree to a bottom element, which in each branch is indicated as a decision point regarding the existence of "PA consequences." Immediately above the consequences decision boxes are the potential critical configurations that can occur. The consequences of a potential criticality include generation of fission products, mobile actinides, heat, water vapor, and radiation. If a criticality event occurs, the impact on performance of the engineered and geologic barriers can be estimated. If the performance of these barriers is unaffected, the consequences are nil. The tree is intended to provide a list of physically possible FEPs associated with post-closure criticality that can be envisioned, not necessarily predictions of FEPs that will occur. The criticality event tree must be used in conjunction with the explanatory text in this document; FEP diagrams are shorthand representations of complex processes and relationships. Those branches that do not obviously lead to failures are not included in the tree.

The FEP-tree organization is intended to provide a perspective on how FEPs may be related and are dependent on each other. Other questions, such as when a branch (scenario) becomes important, how a branch competes with other branches in time and space, and when individual branches are exclusive must be addressed by review, comment, and modification by experts. Additionally, assignment of relative or absolute probabilities of occurrence for the scenarios must also be done before any analysis is complete. WASTE PACKAGE - CONSISTENCY

To illustrate how the tree is constructed and used, and why it branches, the branch involving "drip on containers" will be discussed to the depth of a few alternatives (rather than to the bottom). Because the Criticality Workshop focused on a special problem, this tree begins with the arrival of fluids (groundwater and/or condensate) at the drift. Distinction is made between groundwater and condensate because condensate may or may not contain dissolved constituents (which can affect waste-package corrosion) from rock and the drift liner. How the fluids make their way to the drift is a topic of other investigations. The implicit assumption is that "enough" fluid arrives by whatever means to supply the requirements of any particular branch. In reality, the amount and rate of fluid arrival, as the repository evolves thermally, is currently being modeled.

The topmost FEP "Water (infiltrate/condensate) reaches drift" expresses the otherwise unspecified arrival of enough water. (Please refer to the complete FEP diagram attached to this report.) Depending on the volume of liquid and location of entry into the drift, the tree divides to consider separately the possibilities that liquid drips directly on the container or that the liquid ponds in the bottom of the drift. The latter condition requires a larger volume of fluid and some mechanism to produce a pond on the drift floor. The distinction is made because the location of the dominant waste-package corrosion (top *vs.* bottom), and the times of substantial waste-form mobilization are different. This difference is emphasized by the next two elements in the "Drip" branch, namely "Water drips on waste package" and "Waste-package penetration at top surface." The tree bifurcates to cover FEPs where "Water accumulates in waste package" and the "Waste-package bottom fails, allowing water to flow through." The intent of the former branch is to describe a situation with moderator (water) inside the container.

The tree now splits into three branches based on the relative integrity of the waste form and the interior components of the waste package. Criticality control in the waste package is achieved by inclusion of neutron absorber material, or by limiting the amount of fissile material in the waste package. The tree reflects the assumption that unless the fissile material is separated from the neutron-absorbing materials there will be no criticality (because the original configuration is designed to prevent criticality). For spent fuel, neutron absorbers are most often included in the form of borated steel baskets separating the spent-fuel assemblies. These three branches all express how fissile materials might be separated from neutron absorbers. Each of these branches then continues with a number of sub-branches indicating how the separation of neutron absorbers, based on chemistry, might occur. Several of these sub-branches lead to possible in-package criticality. Additionally, there may be release and mobilization of fissile material, with the possibility of a re-concentration outside of the waste package. Each sub-branch has an extension that allows for further mobilization before a critical configuration occurs. Branch "F" for example, describes mobilization from the container into both the "near-field" and the "far-field" with possible later formation of critical configurations.

It will be noted that several of the branches of the FEP tree are not complete (but end with a "?"). They are possible based on theoretical physical, chemical, or biological principles, but may not be applicable in the Yucca Mountain environment. No evidence for these FEPs have been found in the site environment, so assumptions about their occurrence are very speculative. For example, conjecture about microbial activity causing re-concentration of fissile materials requires assumptions about the post-emplacement environment that have not been established. These incomplete branches are included to provide an exhaustivity to the tree, and will not be considered unless additional experiments or simulation warrant.

CAN WE [illegible] SOMETHING ELSE?

Further elaboration of the tree is left to the readers (or to the readers' questions). This document provides discussion on which, if any, criticality scenarios can occur. The tree itself can be pruned of impossible or incredible events, with the arguments supporting those interpretations being duly recorded. On the complete diagram, the elements describing critical configurations are indicated by color-code as to whether it is an in-package, near-field or far-field problem. All the in-package criticalities are marked with red dots; near-field are coded with blue dots, and far-field with green dots.

2.0 PROCESSES LEADING TO CRITICAL CONFIGURATIONS

As was discussed in the Introduction, the probability of nuclear criticality occurring in sealed, undamaged waste packages is designed to be 0 (i.e., k_{eff} will be less than 0.95, taking into account calculational bias and parameter uncertainty). Therefore, any scenarios leading to in-package, near-field, or far-field critical configurations require the following preliminary processes to occur:

- focusing of water flow onto waste packages
- failure of the waste packages due to water-mediated corrosion
- degradation and/or mobilization of the waste form and internal structures

(Note that disruptions to the repository environment, such as magmatic or seismic events are being analyzed to determine if they could cause failures of intact waste-packages. If this were the case, the scenario discussion that follows might need to be modified. It is likely that the additional impacts of criticality during a volcanic disturbance would be minimal; seismic effects, such as those producing rockfall, could result in failures of otherwise degraded waste packages.)

The following subsections discuss some of the details and assumptions of the preliminary processes for mobilizing fissile material and/or neutron absorbers.

2.1 Water-Contact Modes

The time at which waste packages fail, permitting subsequent change of the environment inside (by allowing exchange of air and water), is an important influence on the formation of potential critical configurations. Time to failure can be influenced by the water-contact mechanisms that result in waste-package corrosion. Furthermore, the repository environment (particularly temperature) and the amount of water available to reach the waste packages can influence the time to failure. Some of the processes include: corrosion rates of metals and waste forms, evaporative concentration of electrolytes, radiolysis of air and water to produce corrosive and dissolving agents, and enhanced localized corrosion and solubilities. These processes are affected most greatly at early times, when temperatures and radioactivity are higher.

2.1.1 Early Breach of Waste Packages

During the first few thousand years after closure it is expected that most water entering the drifts will be vaporized by repository heat. Above a critical humidity level, there will be a moisture film on the waste package that is expected to produce corrosion of the carbon-steel outer barrier, with the rate being dependent on chemistry, temperature, and volume of water available. Because the waste-package inner-barrier material was selected with corrosion-resistance in mind, it is not expected that humid-air corrosion alone will be able to penetrate that barrier. Liquid water containing the electrolytes necessary for localized corrosion, or some other mechanism for failure (such as defects in the welds), are expected to be necessary to penetrate the package. Liquid water may remain in contact with the waste package if the fracture flow is faster than the rate of evaporation. At early times, extended periods of liquid contact are only possible if the container is located under a stable drip that is flowing fast enough to overcome the rate of evaporation. If penetration from any mechanism occurs within about 1,000 years of emplacement, the commercial spent nuclear fuel (SNF) would have sufficient radioactivity to radiolyze the water vapor and nitrogen from the air to rapidly produce aggressive products (e.g., HNO_3, H_2O_2). (Waste-package penetration in less than 1,000 years is not considered likely, given the design effort devoted to ensuring a minimum container lifetime of over 1,000 years.) If present in sufficient quantities, radiolysis products can accelerate the corrosion of internal waste-package structures such as the basket support tubes and criticality-control plates and alter the waste form itself. Pinholes in the SNF cladding may allow interaction of air (O_2) with hot waste, causing rapid oxidation of the waste form on exposed surfaces. If it cannot be demonstrated that the waste-package design is resistant to such early failures, the various types of waste (i.e., commercial SNF, DOE spent fuel, Navy reactor fuel, defense high-level waste (DHLW), and immobilized weapons plutonium) will be evaluated for their response in this environment. Although water vapor may hasten waste-package corrosion, water vapor alone cannot provide sufficient moderation so that thermal criticality can occur. In addition, the ratio of ^{239}Pu inventory within the waste to that of its daughter, ^{235}U, will be maximized at early times.

2.1.2 Later Breach of Waste Package under Dripping

Eventually the waste-package temperature will drop below the vaporization temperature for water (which can vary depending on the concentration of possible solutes), then FEPs that can credibly lead to a criticality event are based on water-induced corrosion of the waste containers. The circumstances thought to be most conducive to producing criticality involve providing sufficient water for moderation, such as by flooding of the waste package. This configuration can develop if the upper portion of a container is penetrated while the lower portion remains intact. A number of detailed scenarios are developed from a partial to total fill of the container based on the possible interaction of the fluid with the contents – waste form, neutron absorbers and structural materials – and the implications of those interactions.

2.1.3 Liquid Ponding in the Drift

If the flow rate of water entering the drift is great enough, if a sufficiently deep depression is created in the floor of the drift, and if drainage through the bottom of the drift is impaired (due to sealing by clays or other fines), then water can collect in the depression and possibly immerse the waste packages. This situation is called ponding in the drift. This partial immersion can induce corrosion at and below the package waterline. Once the waste package fails, water is immediately in contact with the waste form and the waste package internal structural elements (including neutron-absorbing components). As the waste and neutron absorbers are degraded, they can settle in the pool of water in the drift. Distinction is made in the tree between degradation products as solutes and as colloids or larger particles. The FEPs include allusion to the potential effects of bacteria. There has not yet been sufficient study of the possible extent of such phenomena to enable their inclusion in the scenarios.

2.2 Waste-Package Failure

The initial perforations of the waste package will permit entrance of air and water vapor into the interior. Penetration of the waste package permits corrosion and alteration of the interior elements. These perforations can occur anywhere on the waste-package surface. Corrosion products might settle to the bottom of the container and plug the very small penetrations in the bottom waste package, thus permitting a more extensive failure at the top surface to form a water-holding vessel. This water-holding condition is the principal mechanism to provide sufficient moderator to support internal criticality in packages containing SNF. In cases where the waste package has breached in the upper portion, and thus forms a liquid-holding vessel, eventually the bottom will corrode through and release the liquid into the drift. Depending on the length of time the liquid has been in contact with the waste, and the degree of attack caused by the generation of aggressive constituents, there may be a significant amount of fissile material in the effluent from the waste package, which is one of the necessary conditions leading to external criticality.

2.3 Waste-Form Dissolution and Mobilization

Included with the waste form in this discussion are the waste itself and internal structures such as support tubes and criticality control features (collectively called the basket). Zircaloy-clad commercial spent nuclear fuel is quite resistant to aqueous corrosion (CRWMS M&O, 1997f). Factors that can accelerate other forms of Zircaloy corrosion include temperatures above 350 C, which is the lowest possible temperature for the onset of accelerated creep (CRWMS M&O, 1993), presence of SiO_2 in the water, and acids. (Repository and waste-package thermal design intend to keep the peak temperature below 350 C). In addition, pinholes in the cladding can admit oxygen to the UO_2 fuel pellets. As UO_2 oxidizes to U_3O_8, it expands, possibly rupturing the cladding. It is safe to assume that eventually the uranium will be in a higher oxidation state (and thus more soluble) because it will be unprotected by cladding. Other wastes may have less corrosion-resistant cladding or degraded cladding, and may thus fail earlier. The timing of waste-form failure is being investigated in other PA activities.

The corrosion behavior of the borated stainless steel criticality-control plates and the carbon steel tubes in the waste package is of importance to this problem. If the fissile material and the soluble neutron absorbers (principally boron) can be mobilized separately, then criticality control from neutron absorption is lost. Corrosion of the carbon steel tubes produces iron oxides that can accumulate around the spent fuel, providing some neutron absorption and some moderator (water) displacement, thus impairing the conditions for a thermal criticality.

2.4 Transport, Dispersion, and Concentration Mechanisms

Transport in the unsaturated zone (UZ) is mainly by advective groundwater flow through both the rock matrix and fractures. Contaminants may be mobilized into the groundwater either as dissolved species or as colloidal suspensions. As contaminants are transported, they may be reversibly or irreversibly sorbed onto the rock, which retards their movement. (If the chemical characteristics of the flowing water change, the sorbed contaminants can be re-mobilized.) Sorption is generally species dependent, meaning that a plume that originates as a slug of mixed contaminants released from a waste package will eventually contain localized zones of the individual constituents because of the different degrees of retardation of the different contaminants. This phenomenon is called chromatographic separation of the contaminants. Thus, if a fissile species in a contaminant plume were more strongly (or weakly) sorbed than the neutron absorbers, the two would separate. However, this mechanism is far less effective in separating species from distributed contributions from numerous sources (such as leaking waste packages) than from a single slug source. Boron, however, is so poorly sorbed that it may very well become separated from the fissile materials.

Concentration of fissile material can occur by precipitation of dissolved species or by filtration of colloids. Precipitation can occur if there is a change in the chemical state (such as oxidation state) from a more soluble species to a less soluble one. Examples of such processes include the contaminant plume interacting with reducing zones formed by organic matter, the plume mixing with water that has different chemistry, or the chemistry of the carrier plume itself changing. Clays and zeolites, which may be found in localized regions of the Yucca Mountain site, can sorb dissolved fissile materials and trap or filter colloid fissile materials, resulting in their concentration.

Concentration can also occur from topographic or other structural features. A topographic low region of a relatively impermeable zone can permit fissile material to accumulate; dead-end fractures or pinched-out zones can also trap contaminants if water can continue to move through the rock matrix.

The re-concentration mechanisms found at major uranium ore deposits are not known to exist at Yucca Mountain. Specifically, the low solubility of uranium in repository effluents requires long times to achieve significant re-concentration, and there are limited sources of organic materials to provide the chemical re-concentration environment.

Fracture flow in the welded tuffs of Yucca Mountain is now thought to be only weakly coupled to matrix flow. Matrix flow is modeled as being many orders of magnitude slower than fracture flow. Fissile material transported in fractures may be considerably more heterogeneously distributed than that transported through the matrix. As a result, transport in fractures may not represent a significant concentration mechanism.

3.0 OTHER PARAMETERS OF THE CRITICALITY SCENARIOS

3.1 Expected Inventory of Fissile Material

The fissile nuclides of principal interest for long-term criticality are ^{235}U and ^{239}Pu. The initial amounts of these nuclides in the waste forms expected in the repository are summarized in Table 1. With time, the ^{239}Pu (with a half-life 24,100 years) will decay to ^{235}U. The masses per package for commercial SNF containing low uranium enrichment (LEU) and mixed-oxide (MOX) SNF are based on the current baseline waste package designs. The masses for the other packages are based on current conceptual designs (CRWMS M&O, 1997b; CRWMS M&O, 1997a).

Table 1. Fissile nuclides expected in the repository (kg)

Waste form	**^{235}U/pkg.**	**^{239}Pu/pkg.**	**^{235}U total**	**^{239}Pu total**
Commercial SNF (LEU)	100*	60*	635,000	315,000
MOX SNF††	0	200**	0	40,000§
DOE SNF (HEU)	15†	0	2,000§	0
DOE SNF (MEU)	45†	0	2,000§	0
Immobilized Pu	0	200/50‡	0	20,000§

- * Values for the design basis waste (more reactive than 98% of the expected commercial SNF).
- ** Based on the current concept of MOX design for utilization of surplus weapons plutonium.
- § Estimate only, since official design specifications have not been established for this waste form.
- † Planning value, based on preliminary criticality evaluation for aluminum-based SNF and associated waste package. Note, LEU DOE SNF is similar to commercial SNF.
- ‡ Range of possible loadings permitted by the current conceptual designs.
- †† Amounts are uncertain, because this waste form is an alternative considered for disposal of the excess weapons plutonium.

The commercial SNF (CSNF) is part of the legislative mandate for the repository; the legislative mandate has been interpreted to include other waste forms such as DOE SNF and the spent fuel from Navy reactors (DOE, 1984). Not shown is the defense high level waste glass (resulting from reprocessing). The amount of fissile material in the DHLW is too small by itself to pose a significant criticality threat. The fissile content per waste package for the Navy spent fuel, although of higher enrichment, is about 25% less than that for commercial SNF, and the total fissile mass is expected to be less than 61,000 kg.

Whether a given mass of fissile material will become critical depends on the geometry, the presence of neutron absorber material, and the amount, and type. of moderator. Therefore, it is not possible to specify a critical mass for these waste forms without giving specific configurations. Nevertheless, it is useful to consider the masses in Table 1 with respect to a mass of fissile material that could become critical under the most conservative conditions. The fissile capability of ^{239}Pu is approximately 20% greater than that of ^{235}U, although the actual difference will depend on the amount and type of moderator, with the strongest advantage of Pu coming with the higher energy neutron spectrum (epithermal) characteristic of moderation in tuff. To the approximation of this discussion, the two isotopes can be considered to behave the same neutronically, and will simply be referred to as fissile material. Their chemical behavior (solubility, adsorptivity, etc.) will be quite different.

Three of the waste types (commercial SNF, MOX SNF, and DOE SNF) contain between 20 and 50 times as much ^{238}U as ^{235}U. Since the ^{238}U has strong neutron absorbing behavior, minimum ^{235}U mass that could support criticality for these three waste types is between 50 and 100 kg. Thus, a single waste package containing commercial SNF is not expected to be able to go critical because of the absorption of fission neutrons by ^{238}U. In contrast, the fissile material in the waste forms without much ^{238}U (immobilized plutonium and HEU DOE SNF) could theoretically support criticality with only a mass of 15 kg under the worst-case conditions believed to be possible in the repository. (With an ideal spherical geometry, a homogeneous mixture of fissile material and water, and with water reflection and moderation, a mass of less than 1 kg of plutonium or HEU could support criticality.) Waste-package design restrictions may limit the amount of HEU or Pu in containers so that there may be insufficient amounts to provide a critical mass of these elements.

The masses of fissile material per package given in Table 1 are comparable to, or somewhat greater than these worst-case criticality support masses, but the corresponding waste package designs and concepts have been shown to protect from criticality because of the large amount of neutron-absorber material that is incorporated into the design. For criticality to occur in the waste package, nearly all the absorber material would have to be removed from the waste package, without removing any significant amount of the fissile material, a very unlikely circumstance.

A criticality event (even up to 10,000 years' duration) generally consumes so little fissile material that a criticality at one time does not preclude another one at a later time from the same source material (CRWMS M&O, 1996b). However, the limited amount of fissile material in a waste package would preclude outflow from a single package supporting criticality at more than one location at a time.

3.2 *Interactions Among Waste Types*

Although the majority of the repository waste, commercial SNF, has been extensively characterized, the presence of other waste types can change the nature of the criticality problem. Not only mixtures of waste types within a single container must be considered, but also the potential thermal and chemical influences of nearby degraded waste packages. For example, the glass encapsulating DHLW can alter to clays, which could significantly alter the transport characteristics of contaminants, and also could change the criticality parameters. The presence of either HEU or plutonium can change the parameters of commercial SNF critical configurations. Waste-package design and fissile loading for additional waste forms will include these considerations.

4.0 DISCUSSION OF CRITICALITY FEPS

The FEP diagram provided with this report is based on the issues developed at the criticality workshop. It provides a progression of FEPs from the condition of water entering the drift to potentially critical configurations occurring in-package, in the near field, and in the far field. To most effectively analyze potential critical configurations, readers should follow paths in the FEP diagram from the entry point to the decision points labeled "PA Consequences?." As the tree is traversed, the analyst can identify the particular environmental or nuclear parameters necessary to develop a potentially critical configuration. This systematic approach will aid in selecting potential critical configurations that should be further analyzed. The complete diagram is provided as an attachment to this report; fragments of the tree are shown as figures to emphasize discussions in the text.

The FEP diagram starts with water entering the drift and interacting with waste packages (Figure 1). One branch follows the FEPs when the container surface is directly contacted by dripping water for extended periods of time. The other branch is for partial immersion of the waste package from standing water in a drift. Extended periods of liquid water contact are thought necessary for the localized penetration of the corrosion-resistant inner waste-package material. Extended water contact may occur either at very early times during the thermal pulse, or at later times when the containers have cooled to below the boiling temperature. Early liquid contact during the thermal period is different from later liquid contact mainly in the rates of the processes that may lead to criticality and is thus not broken out separately in the diagram.

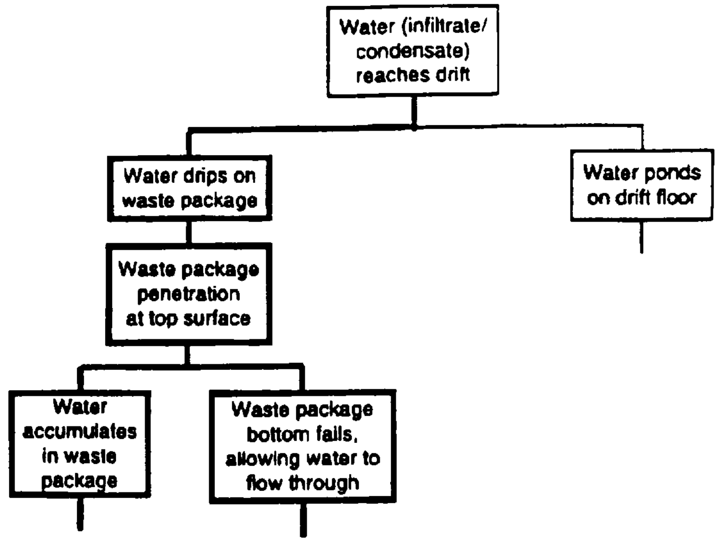

Figure 1. Initial FEPs leading to waste-package failure.

4.1 Waste-Package Degradation

The branch continues with conditions where the upper portion of the waste package is penetrated before the bottom is breached. As a result of this corrosion failure, water can accumulate in the waste package, providing neutron moderation, as well as providing a mechanism for corroding and moving the fissile materials relative to the neutron absorbers. This "bathtub" failure mode is illustrated in Figure 2. The tree next branches to indicate either prolonged water accumulation or corrosion of the waste-package bottom, which permits the water to flow through the package.

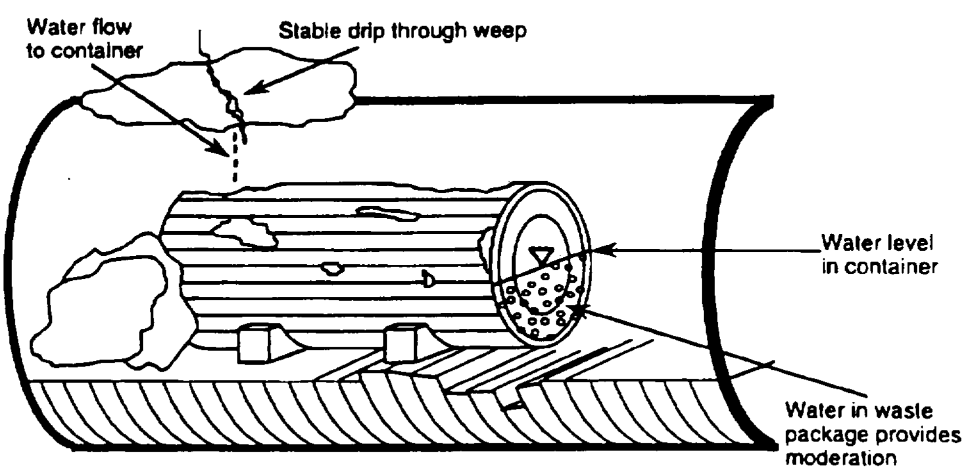

Figure 2. Illustration of failure of waste-package top.

4.1.1 Accumulation of Water in the Waste Package

The tree divides according to the relative rates of degradation of the waste form and/or waste-package criticality-control structures. Depending on the type of waste and the type of waste-package internal structures, there can be significant differences between the rates of degradation.

4.1.1.1 FEP-Tree Segments IP-1a and IP-1b

This tree segment illustrates the primary FEPs that could lead to in-package criticality for waste forms that degrade faster than the waste-package internal structures (Figure 3). These waste types are primarily the aluminum-clad DOE SNF that is co-disposed with DHLW. The left-hand branch, leading to configuration **IP-1a**, illustrates critical configurations that could occur if the reactor fuel assemblies in the waste became more reactive due to degradation in place. Corrosion of the aluminum-clad SNF produces a gelatinous degradation product that retains water (CRWMS M&O, 1997e); additionally, the fissile material is more homogenized when the cladding degrades.

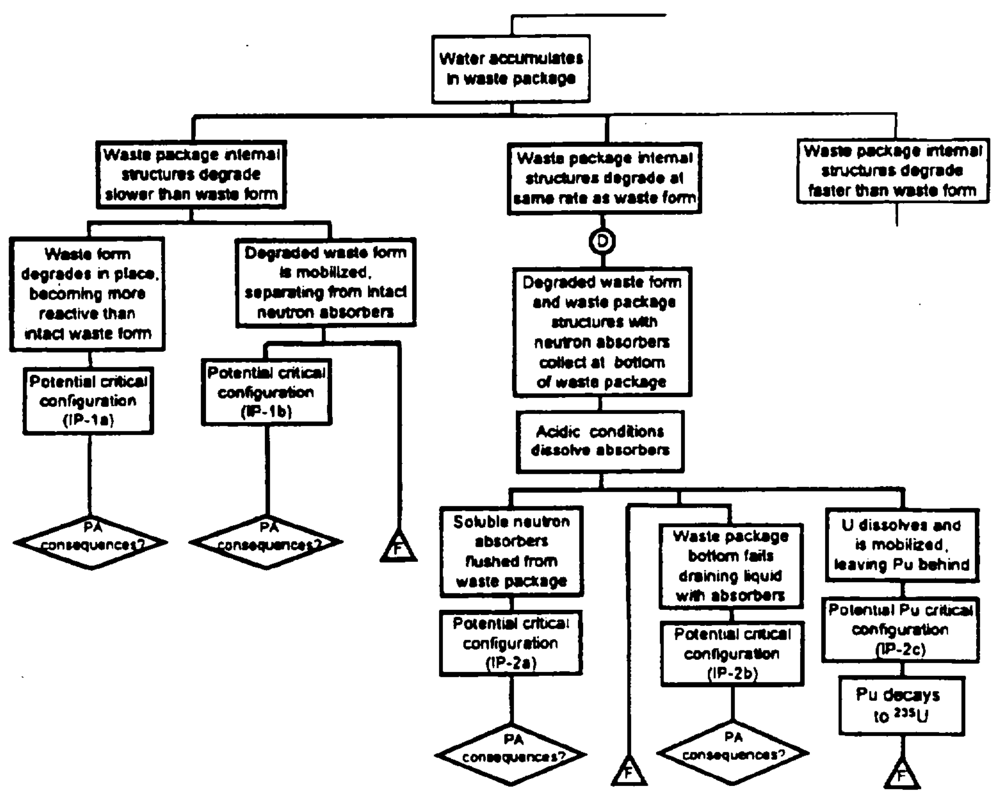

Figure 3. Critical configurations for waste-form degrading faster or equal to rate for waste-package internals.

If instead the waste form degrades and the fissile material is mobilized, the fissile material can become separated from the neutron absorbers remaining in the internal structures. Configuration **IP-1b** assumes there is sufficient moderating water present to permit thermal criticality of the fissile material in the bottom of the waste package. The branch of the tree (labeled "F") leads to potential near-field and far-field critical configurations, which are discussed in later sections.

4.1.1.2 FEP-Tree Segments IP-2a – IP-2c

This tree segment (also labeled "D") illustrates scenarios leading to potential in-package critical configurations where the waste and internal structures degrade at similar rates (Figure 3). Glass or ceramic waste containing plutonium in a pour canister is an example of such a configuration, although other waste forms may eventually follow this branch. Glass degrades in the presence of oxygen; as it does, it turns to clays which can hydrate and become mobile. If the fissile material and absorbers collect at the bottom of the waste package, then configuration **IP-2a** illustrates the case of a thermally critical configuration that occurs after the neutron absorbers dissolve and are removed by water flushing them away. The neutron absorbers used in Pu-glass include both borates and gadolinium compounds. (The soluble borates are included to make the glass more workable and act only incidentally as neutron absorbers.) Gadolinium compounds are insoluble for pH values greater than 6; under acidic conditions they can dissolve and be flushed away. Configuration **IP-2b** occurs if the waste-package bottom fails, allowing water flowing through the waste package to flush the soluble absorbers away. For this configuration to occur, the fissile material must be either HEU or plutonium in order for it to be able to go critical with little or no water. The moderating water is contained in the clays from the DHLW glass/ceramic degradation. If the waste contains both uranium and plutonium, then the greater solubility of the former may result in transport of the uranium, leaving the plutonium behind. If removal of the neutron absorbers occurs (as has been discussed above), then a potential critical configuration (**IP-2c**) for plutonium can occur. Eventually the ^{239}Pu decays to ^{235}U. The uranium can be mobilized (as shown by the path leading to branch "F"). A far-field critical configuration involving ^{235}U is discussed below.

FAST?

4.1.1.3 FEP-Tree Segments IP-3a – IP-3d

This branch assumes that the waste form is corrosion resistant, and the waste-package internal structures degrade first (Figure 4). Such an assumption only applies to specific reactor fuels, and is most applicable for SNF (since it is clad with Zircaloy or stainless steel, which are much more corrosion resistant than the steel of the waste-package basket). The waste packages for SNF are designed to provide three levels of neutron absorption — no neutron absorbers for spent fuel with reactivity (as measured by k_∞) < 1.0, borated steel absorber plates for spent fuels with $1.0 < k_\infty < 1.13$, and Zircaloy-clad absorber rods for spent fuel with $k_\infty > 1.13$. (A value of k_∞ of 1.13 corresponds here to a k_{eff} of approximately 0.95 – the NRC regulatory maximum.) This discussion focuses on packages with the boride–steel absorber plates.

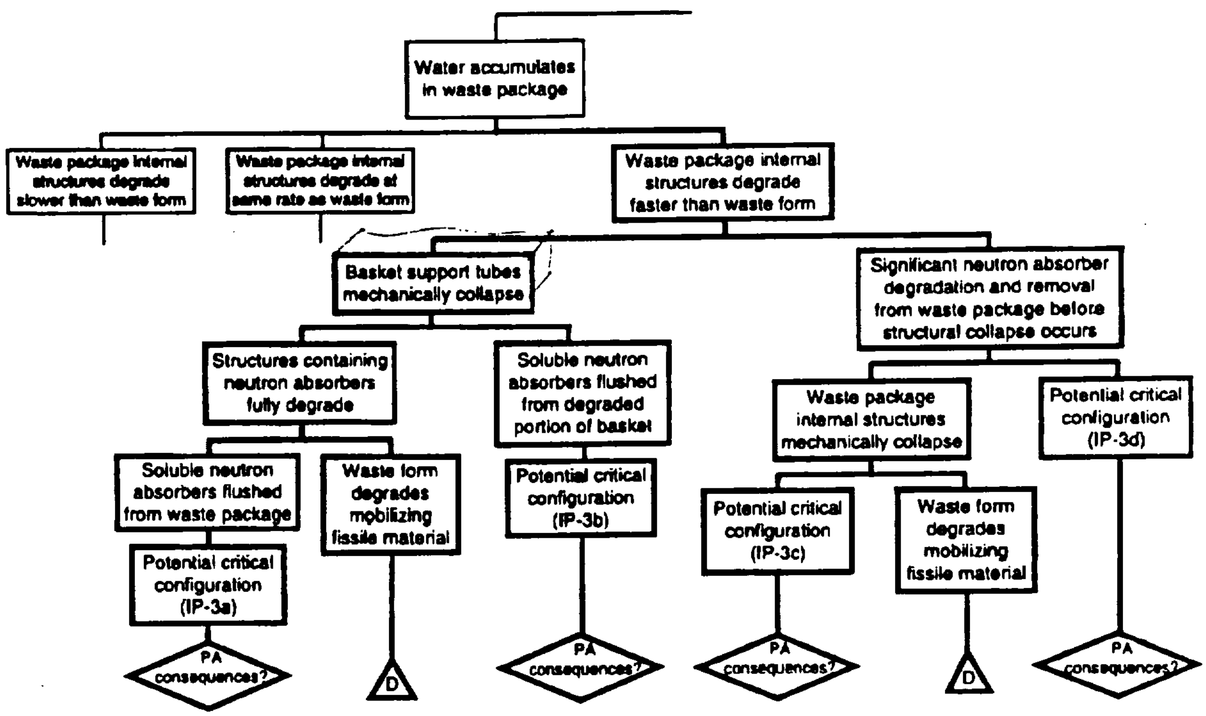

Figure 4. Critical configurations for waste-form degrading slower than waste-package internals.

The left-hand sub-branch assumes the basket mechanically collapses. Figure 5 illustrates the succession of stages of collapse of the waste-package internal structures. Configuration **IP-3a** illustrates potential thermal criticality if the absorber structures completely degrade. The basket corrosion products would include insoluble iron oxides and oxy-hydroxides that would settle between the fuel rods to the bottom of the container. The fate of the boron could either be direct dissolution to soluble borates or could involve liberation of small chromium boride particles that could settle to the bottom of the container before final dissolution to soluble borates. If the boron is directly dissolved, it may be removed from the container as additional water enters the container and flushes the dissolved species away (the overflowing bathtub scenario). If it settles to the bottom of the container, it is removed from the fissile material providing the first step necessary for criticality. If the mechanical integrity of the waste form is adversely affected, then the tree leads to branch "D." Note that this process does not apply to commercial SNF, which can only go critical with the fuel rods in a near-optimal spacing. The consolidation implied in this scenarios excludes the moderator to the extent that only highly enriched fuel (of which stainless steel-clad SNF is only a small fraction) can support criticality. If the basket and fuel-assembly spacers only partially degrade (as might be the case for Zircaloy-clad CSNF), sufficient absorbers may be flushed away that a critical configuration may form with the fissile material in its initial configuration (**IP-3b**).

NOW THIS ONE IS DOUBTFUL FOR CSNF.

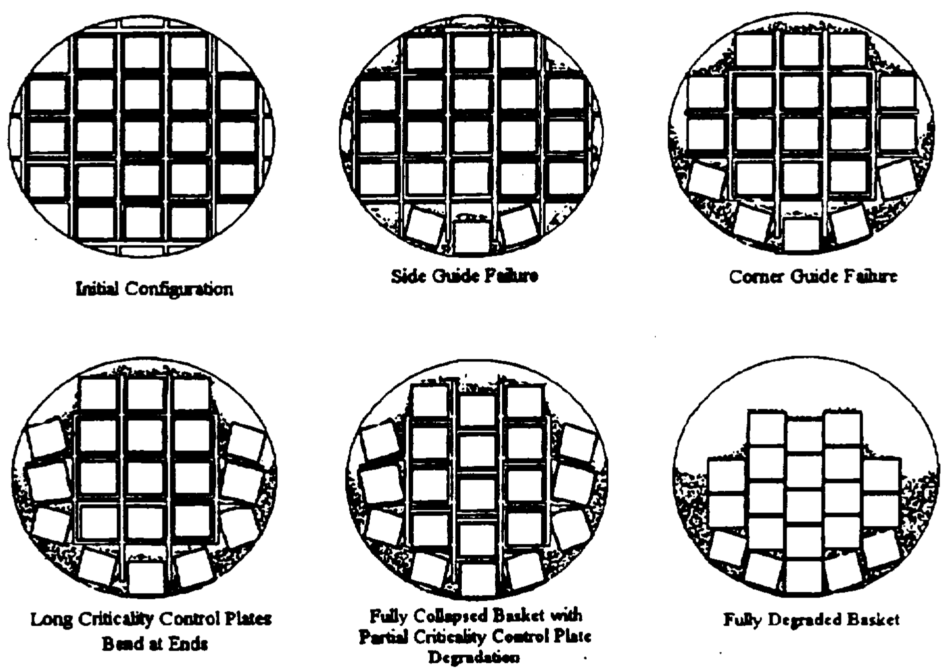

Figure 5. Stages of collapse of waste-package basket structure (after CRWMS M&O, 1997f).

Configurations **IP-3c** and **IP-3d** indicate potential criticalities resulting from accelerated removal of neutron absorbers from the basket before it mechanically collapses. These events are most likely to occur if the multipurpose container (MPC) is used as a waste package. The neutron-absorbing structures of the MPC are made of a boron-loaded aluminum material (Bor-Al), and the initial fuel-assembly spacing is designed to be larger than the optimum for criticality. The MPC is not being currently considered as a design option. Configuration IP-3c considers the case where the fuel assemblies consolidate to the optimal spacing for criticality as a basket collapse after absorber removal. In configuration IP-3d, absorbers are removed but collapse does not occur.

If the waste form itself degrades at this point, the FEPs are substantially the same as those shown for branch "D" (discussed above). It should be noted that the reactivity of SNF decreases somewhat if the fuel-pin spacing decreases due to mechanical collapse of the fuel-assembly spacers, so the likelihood of a critical configuration from this fissile-material source may be lower than for the IP-2a and IP-2b branches as they apply to Pu-glass.

4.1.2 Water Flow Through the Waste Package

This branch considers the waste-package degradation mode where both the top and bottom are penetrated, thus permitting water to flow over the waste and through the package. As with the bathtub case, the tree identifies three possible alternatives among the relative rates of degradation of the waste form and the waste-package structures. Because there may not be as much water present in the waste package (as compared with the previously discussed "bathtub" branches), the potential critical configurations may require different types of fissile material or waste-package construction to occur. The branches are shown in Figure 6.

ARE THESE ALL THERMAL CONFIGURATION RELYING ON HYDRATED CORROSION PRODUCTS TO MODERATE? IF SO, NEED TO STATE CLEARER.

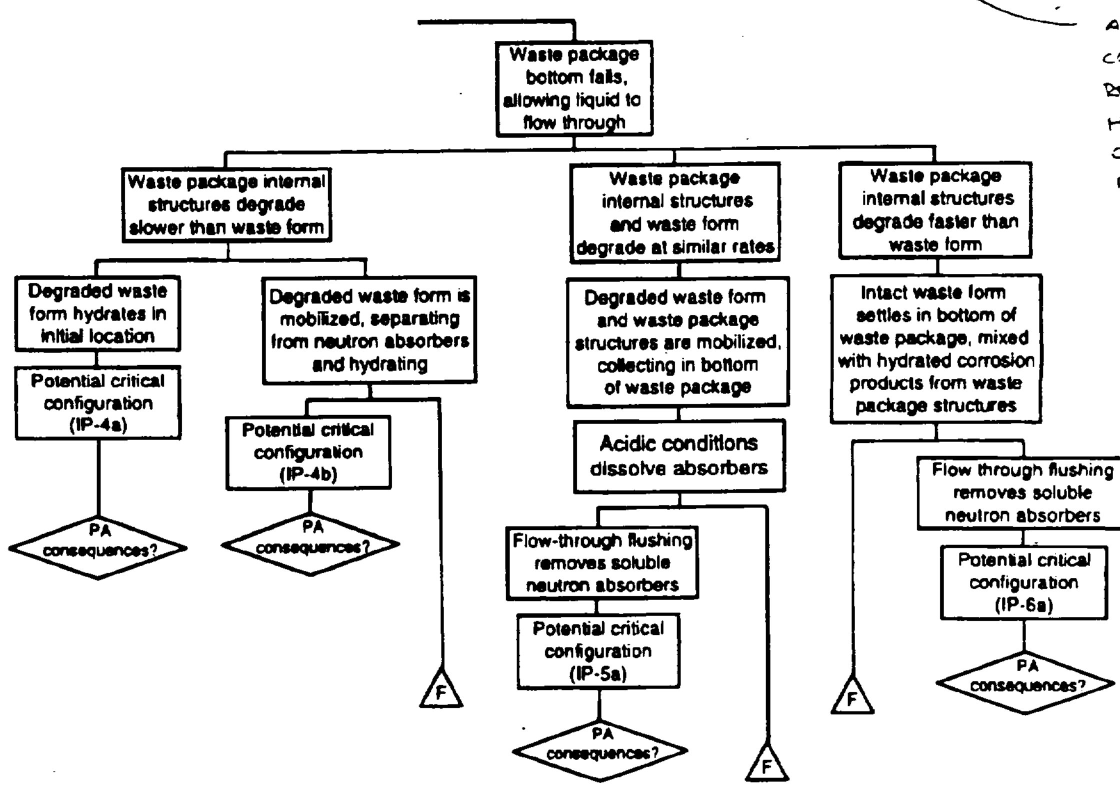

Figure 6. Critical configurations for flow-through waste-package failure modes.

4.1.2.1 Tree Branches IP-4a and IP-4b

In the case where the waste form degrades faster than the waste-package internal structures, the resultant corrosion effects important for criticality analyses include the formation of hydration corrosion products in the waste. The most likely waste form that can undergo such relatively rapid degradation is aluminum-clad spent fuel co-disposed with DHLW. Potential critical configuration **IP-4a** illustrates the situation where the hydration occurs without having the waste form mobilize. If the fissile material and hydrated corrosion products do collect elsewhere in the waste package, potential critical configuration **IP-4b** is applicable.

4.1.2.2 Tree Branch IP-5a

Excess weapons plutonium, immobilized in glass (or ceramic) in the can-in-can emplacement alternative, can be mobilized as the glass degrades. The glass generally forms (hygroscopic) clays that can be intimately mixed with plutonium particles and neutron absorbers in the waste package. As discussed in Section 4.1.1.2, the neutron absorbers designed in to the waste forms are generally less soluble than the fissile material. However, under low pH FAST? conditions, some of the absorbers could dissolve. If the soluble absorbers are flushed from the clay-plutonium mixture by the groundwater passing through the waste package, potential critical configuration **IP-5a** could develop.

4.1.2.3 Tree Branch IP-6a

Lastly, Zircaloy-clad spent reactor fuel is likely to remain intact for longer than the waste-package internal structures, especially for the MPC design. As the internal parts degrade, the fuel pins can consolidate in the bottom of the waste package. Hydrated corrosion products from the waste-package internal structures can include iron oxides or aluminum hydroxide from the MPC internal structures. As groundwater flows through the waste package, dissolved neutron absorbers can be removed, potentially creating a critical configuration (**IP-6a**). FAST? OR IS IT HYDRATED

4.2 Fissile-Material Re-Concentration In Near Field

After a waste package has failed, any degraded waste inside can eventually be mobilized and thus transported outside the containers. Potential critical configurations can then occur in the drift or the repository engineered structures (i.e., the near field). These critical configurations are discussed in this section (Figure 7). Two main branches of the FEP diagram are discussed — where the waste package has initially corroded at the top and subsequently at the bottom (Section 4.2.1), or where water has collected in the drift outside the waste package and has corroded it to failure from below in the immersed portions (Section 4.2.2). In the former case, depending on whether the water has accumulated in the waste package or flowed through can influence the nature of the critical configuration in the near field.

The materials first encountered by effluent from the waste packages is either concrete or crushed tuff invert, plus corrosion products from degraded waste packages and waste forms. These materials can react with the effluent to concentrate fissile materials. Reactants include carbonates from the tuff or concrete, iron corrosion products, zeolites and clays, and other minerals.

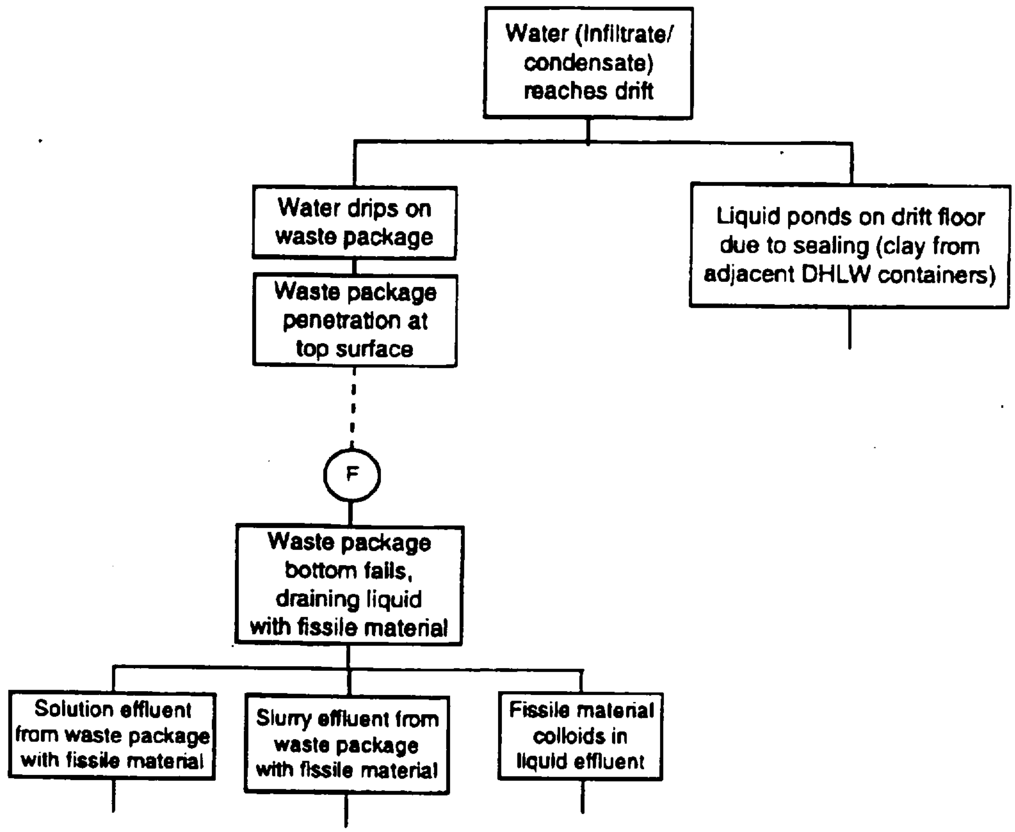

Figure 7. FEPs leading to near-field critical configurations.

4.2.1 Failure of the Waste-Package Bottom after Failure of the Top

When the bottom of a waste package that contains water and dissolved waste corrodes through, the liquid and possibly solids can flow onto the drift floor and into the invert. This is illustrated in Figure 8. This branch of the FEP tree (branch "F") is shown as following from the upper branches in which the waste form and/or basket have degraded in a waste package. The physical and chemical environment in the invert (crushed tuff and/or concrete) may permit separation of fissile material from neutron absorbers and concentration of the fissile material. Such conditions may result in near-field critical configurations if it can be shown that the accumulated material will exceed any of the single-parameter limits (such as mass, thickness and diameter) for a specified enrichment. Branches of the tree are based on whether contaminants are in solution, are colloidal suspensions, or are slurries.

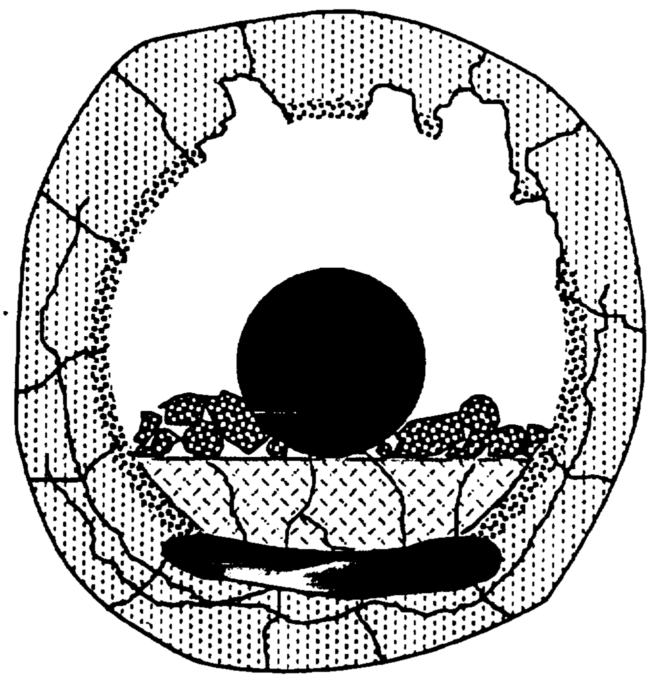

Figure 8. Illustration of near-field critical configurations.

4.2.1.1 FEP-Tree Segments NF-1a and NF-1b

If the waste-package effluent contains fissile material and neutron absorbers in solution, then re-concentration can occur by precipitation and/or sorption. The fissile solute most in abundance is uranium. Uranium sorbs onto iron oxy-hydroxides and onto clays and zeolites, and the amount of sorption is dependent on the pH. A high-pH solution of fissile material and absorbers will sorb onto materials likely found in the drift, but can de-sorb as the pH reverts to neutral. A continuous or distributed source of fissile solutes can result in a concentration of fissile material in the invert materials. This may result in sufficient concentration that a thermally or epithermally critical configuration (**NF-1a**) may occur (Figure 9).

If the water transporting and concentrating the fissile material is insufficient to provide moderation of a thermal criticality, and sufficient fissile material for an epithermal criticality has accumulated, then a silica-moderated epithermal critical configuration may occur. An epithermal criticality requires a greater concentration of fissile material, but the water available to do the concentration is less.

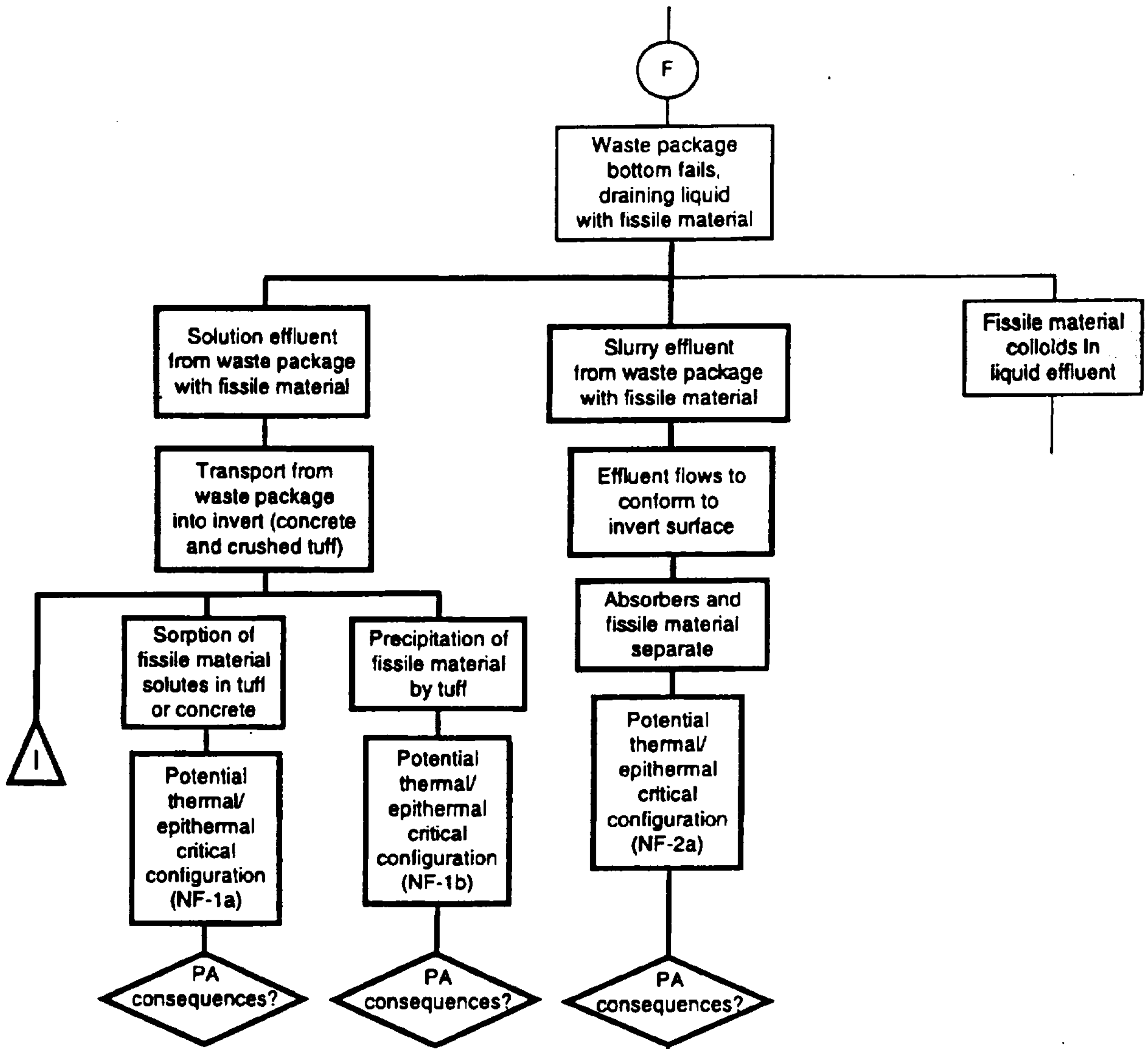

Figure 9. FEPs leading to near-field critical configurations for fissile solutes and slurries.

Waste-package effluents can range in pH from highly acidic to highly basic; at either of these extremes the uranium solubilities are greater than at neutral pH values (CRWMS M&O, 1997a). Interaction with tuff (which has a more neutral pH) can therefore precipitate uranium. Concrete normally has a high pH, so it is less likely to precipitate uranium from high-pH solutions. If the fissile material precipitates onto the tuff invert materials, this may provide sufficient concentration for a thermally or epithermally critical configuration (**NF-1b**). The pH of the tuff can be altered as it interacts with the solution to the point that it will no longer precipitate uranium. This can limit the concentration of fissile material that can accumulate by this mechanism. The water available to moderate a critical configuration is assumed to be both from the waste package effluent and non-effluent (i.e., uncontaminated with fissile materials). FEP tree branch "I" shown in the figure leads to far-field potential critical configurations for fissile solutions.

4.2.1.2 FEP-Tree Segment NF-2a

If the waste package contains Pu-glass or ceramic, then degradation of the glass creates a clayey mass that can provide a slurry-like mixture. The significance of clay is that it may retain sufficient water for moderation, so that criticality is possible without liquid water. The clayey mass is assumed to contain fissile materials and both soluble absorbers, such as boron, and lesser amounts of insoluble absorbers, such as fission-product rare earth elements. If the aqueous environment becomes acidic, additional water will leach the absorbers and transport them away, providing a mechanism for separation of fissile and absorber materials (**NF-2a**) (also shown in Figure 6).

4.2.1.3 FEP-Tree Segments NF-3a – NF-3c

For the case that waste-package effluent contains fissile materials in colloidal suspension three near-field branches are possible (Figure 10). Configuration **NF-3a** illustrates potential criticalities that develop from concentration of fissile material by filtration through corrosion products from the waste package. If the colloids are transported through fractures in the invert then they may undergo hydrodynamic separation and concentration in the fractures. This may lead to epithermal or thermal criticality (**NF-3b**), as described for configuration NF-1a above. Lastly, if the concrete in the invert degrades in such a way that it greatly increases its permeability and flow-path tortuosity, it may provide an alternative environment for colloid filtration or sorption that results in an epithermal or thermal critical configuration (**NF-3c**). Branch "J" leads to potential far-field critical configurations.

4.2.2 Failure of the Waste-Package Bottom First

If there is sufficient water flow into the drift, and if drainage from the drift is impaired by formation of a depression with the subsequent plugging/sealing of drainage by fractures, then water can collect and partially immerse the waste packages, as illustrated in Figure 11. A basin can form in the invert by thermally induced buckling of the floor, by rockfall dams, or by other stress-relief movements (see Figure 12). In this branch of the tree, corrosion of the waste package is assumed to be faster from the waterline downwards than on the upper portion. Thus, failure of the waste package permits mobilized fissile material to readily leave the waste package, and potentially collect in the drift. Depending on the extent of sealing of the basin by clays or other fines, water and solutes/colloids/particulates may be contained in the basin, or the bottom may act as a filter.

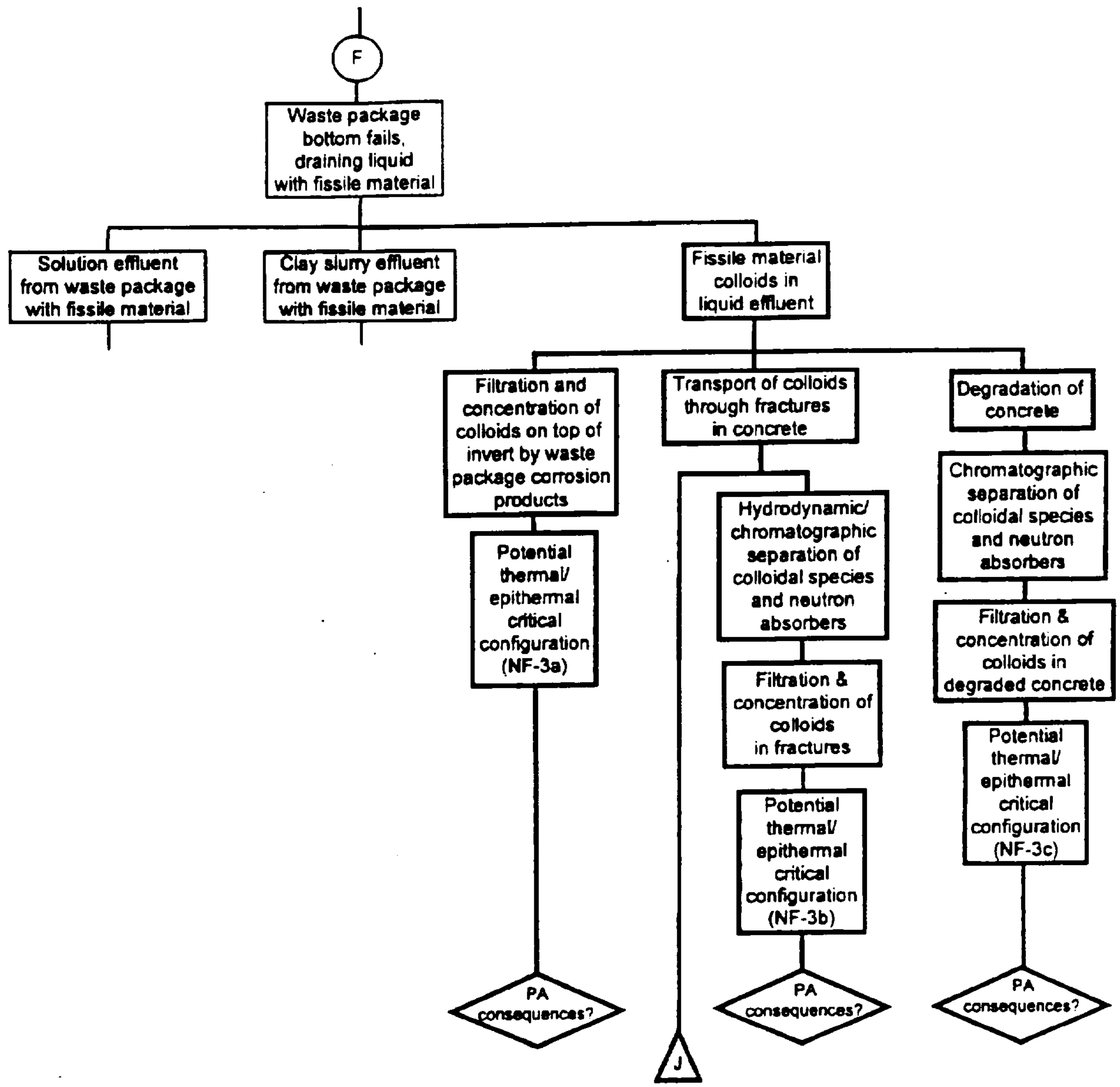

Figure 10. FEPs leading to near-field critical configurations for fissile colloids.

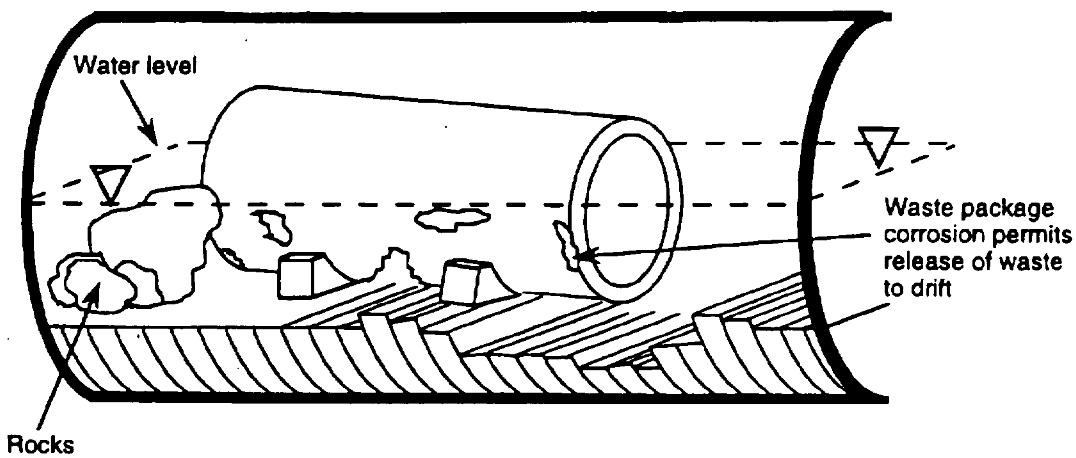

Figure 11. Illustration of failure of waste package from bottom.

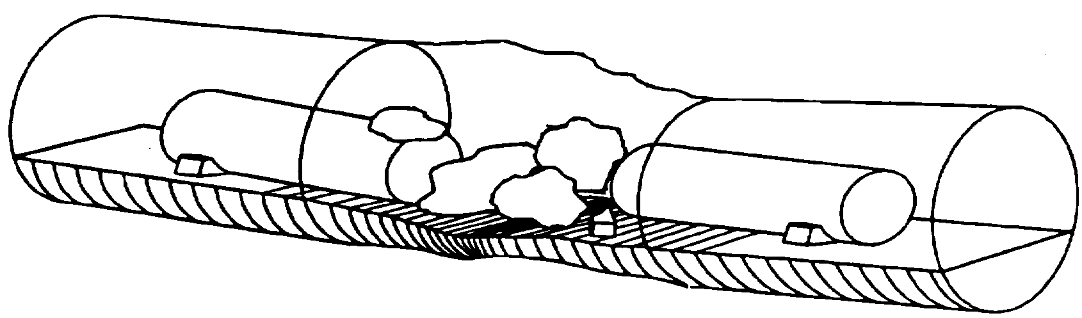

Figure 12. Illustration of ponding conditions in drift.

If the breach in the bottom of the waste package is large enough, fissile particles larger than colloids may spill from the container along with other corrosion products. The resulting sludge would be expected to behave as a porous medium that could retain significant water. If the resulting mass of sludge is large enough and if the soluble absorbers have been leached away, a thermal or epithermal criticality may occur. At late times, when the container is severely degraded, the distinction between an in-package and this near field criticality will become similar.

4.2.2.1 FEP-Tree Segments NF-4a – NF-4e

This tree segment illustrates near-field potential critical configurations for ponding scenarios (Figure 13). If the basin is sealed, then fissile-bearing materials can collect at the bottom of the pond. An epithermal/thermal critical configuration (**NF-4a**) can then develop. At the extreme limit, the entire contents of the waste package could be dumped into the drift, providing the same amount of fissile material as would be available in an in-package critical configuration. If the fissile deposit is stratified along the bottom of the basin, a disturbance such as a falling rock may mix the water moderator and the fissile material and provide critical configuration **NF-4b**.

In contrast, if the basin acts as a selective filter, the more mobile uranium may pass through the bottom, leaving plutonium behind (branch "E"). This may form potential critical configuration **NF-4c**. Configuration **NF-4d** is similar to NF-4b, where stratified Pu is mixed with a moderator by a disturbance. Lastly, critical configuration **NF-4e** could occur if the ^{239}Pu decays to ^{235}U.

The actions of microbes in the pool on contaminants are unknown. Microbes could fix actinides in their metabolic systems; decaying microbial deposits could provide a reducing environment that could precipitate uranium. Microbes can also utilize uranium as an electron acceptor in redox reactions, resulting in reduction (and thus precipitation) of the uranium. This branch of the FEP diagram will be expanded if further information becomes available.

IN THE END, BOW

4.3 *Fissile Material Re-Concentration in the Far Field*

Fissile-material solutes or colloidal suspensions can be transported from the waste package, through the invert, and into the repository host rock. Transport may occur in a "carrier plume" — groundwater that has been significantly altered by interaction with the repository. The pH, temperature, and chemical species of the carrier plume can differ from those of infiltrating groundwater. Both solutes and colloids can be transported (illustrated by FEP tree branches "I" and "J"). During transport, separation of neutron absorbers from fissile materials can occur by hydrodynamic and sorptive processes. The primary consequence of transport will be dilution of the contaminants in the groundwater by diffusion, dispersion, retardation, or mixing. Formation of critical configurations therefore requires re-concentration mechanisms.

As discussed in CRWMS M&O (1997g), the re-concentration processes for fissile materials are essentially those for epigenetic (deposited after the host rock) ore-body formation. Because of the low solubility of plutonium and the long time periods, consideration is primarily given to uranium ore-body formation. The assumption is that the relatively immobile plutonium will have sufficient time to decay to uranium prior to transport.

REMEMBER, YOU HAVE A LOAD OF U^{235} IN MOST PACKAGES ONLY A FEW HAVE HEU. THUS ON AVG HAVE SUFFICIENT (LIKELY) ABSORBER HOW FAR FOR HEU PACKAGES.

PU-DECAY NEEDS QUESTION.

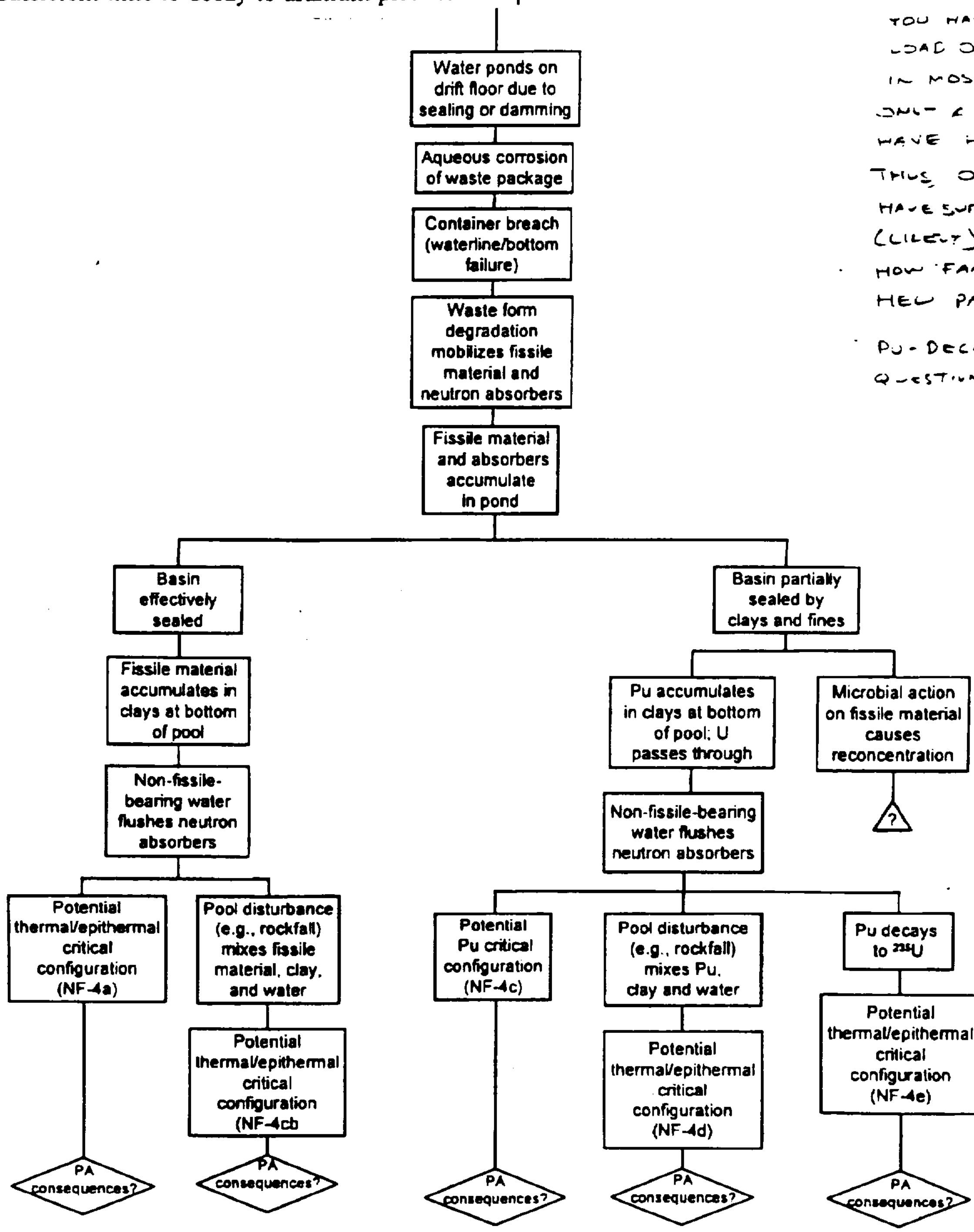

Figure 13. FEPs for near-field critical configurations due to waste-package failure from the bottom.

Uranium is relatively soluble in its oxidized (+6) state, and quite insoluble when reduced (+4 state). A reducing environment (or the presence of abundant oxidizable elements, such as vanadium) is essential to the precipitation of uranium. Naturally occurring ranges of pH (i.e., 7 to 8.5) are not sufficient to provide an environment that will precipitate uranium. The three types of epigenetic ore-deposit formation processes most applicable to Yucca Mountain are unconformity, sandstone, and calcrete-type deposits.

I'M CONFUSED ON PG 2
U SOLU. ARE GEN. @ HIGH & LOW PH EXT.

Unconformity deposits develop when oxidizing groundwaters dissolve uranium and transport it as the +6 oxidation state. If the uranium solution reaches a permeable sandstone or conglomerate above an unconformity, then reducing agents (e.g., hydrocarbons or hydrothermal solutions) in groundwater that are moving upward along faults from the basement rock and through the unconformity contact boundary can reduce the uranium to the +4 state and cause precipitation.

DEPENDS ON SORPTION DEPT. IF ABS, WILL MIX W/ OTHER U. IF LITT WILL PASS

Sandstone deposits occur because of either organic or inorganic reducing agents present in an area of relatively high permeability. As a secondary mechanism, sorption of uranium onto zeolites or clays also occurs in sandstone-type deposits. Often these deposits occur at roll fronts. The reducing agents can be organic materials (organic debris, buried logs, lignite, etc.) or inorganic (iron- or sulfur-based minerals); sorption can occur on clays and zeolites.

Calcrete-type deposits are near-surface deposits that occur where evaporation exceeds recharge, such as playa lakes. As water evaporates, incongruent precipitation of the solutes changes solution pH and the oxidation state of other minerals in solution. Oxidation of vanadium as uranyl-ion bearing water evaporates is a known mechanism to cause uranium precipitation. Vanadium is not known to be abundant in the Yucca Mountain region, so this mechanism for calcrete formation may not be of great importance. Evaporation alone may be able to precipitate some other uranium minerals also.

4.3.1 Fissile Material Re-Concentration in the Unsaturated Zone

If fissile solutes or colloidal suspensions are not trapped in the near field, they can be transported further away from the repository. Transport in the unsaturated zone (UZ) occurs in the rock matrix or the fractures. The re-concentration mechanisms associated with these two types of transport are different, as discussed below.

4.3.1.1 FEP-Tree Segments FF-1a – FF-1c

Because plutonium is relatively insoluble in groundwater (compared to uranium), this branch is most applicable to uranium transport and re-concentration. Sorption that can occur during UZ transport can result in separation of the neutron absorbers from the uranium; changes in groundwater chemistry to reducing conditions will precipitate the uranium. Tree branch "I" illustrates solute transport and subsequent re-concentration by precipitation or sorption (see Figure 14). Potential critical configuration **FF-1a** assumes that localized precipitation (such as in fractures) could occur if the chemistry of the carrier plume is changed by interaction with country rock. As was discussed in Section 4.2.1.1, if a high-pH solution of uranium in the carrier plume is neutralized by the country rock, the uranium will precipitate.

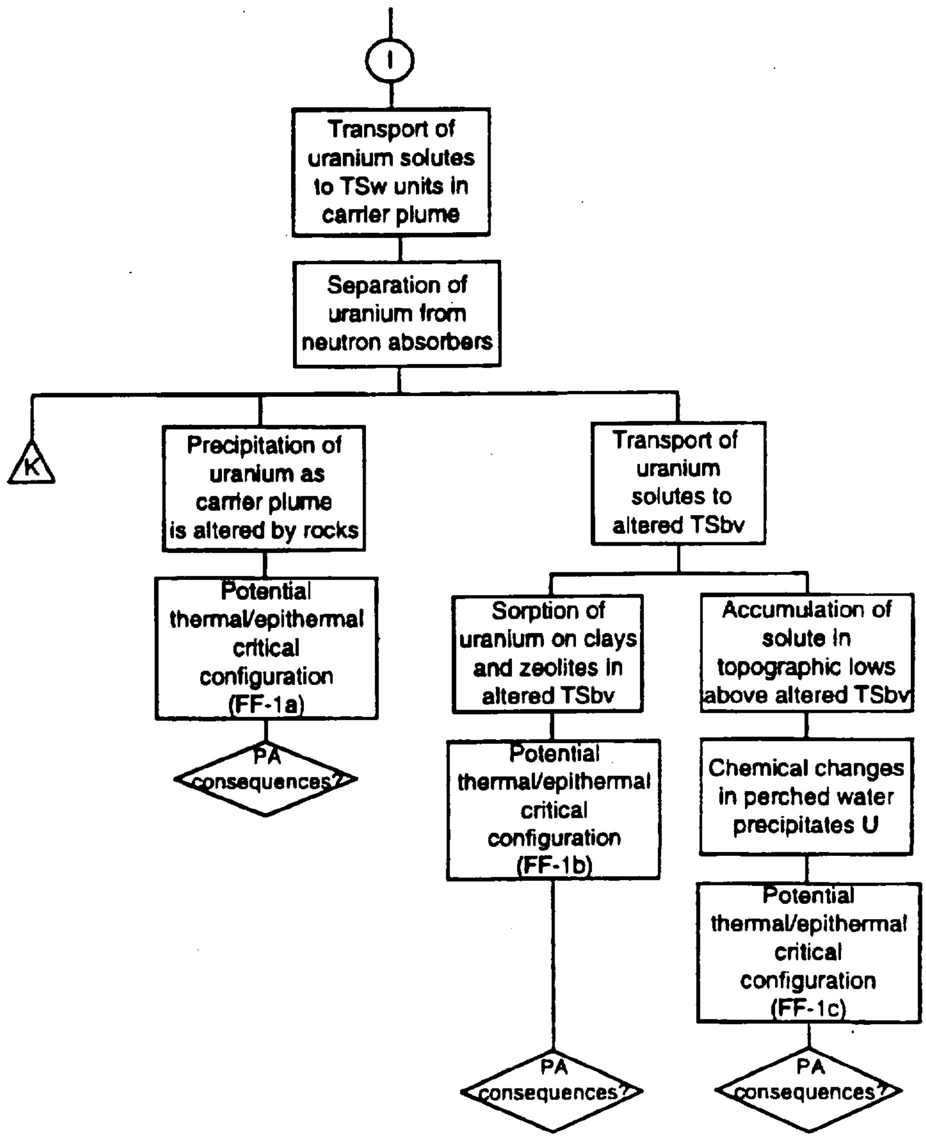

Figure 14. FEPs for far-field critical configurations for fissile solutes in the unsaturated zone.

Repository-induced hydrothermal changes in the Topopah Spring basal vitropyhre (Tptpv3 – also known as the TSbv unit) can generate clays that can reduce the permeability of that unit. The clays and zeolites of the TSbv can provide sorption sites for uranium, as illustrated in **FF-1b**.

Topographic depressions in the upper boundary of the altered TSbv may provide locations where uranium solutes and water can accumulate (i.e., a perched-water body). If chemistry changes occur in the perched water, uranium will precipitate and may result in a potential epithermal/thermal critical configuration (**FF-1c**). This is illustrated in Figure 15. In terms of similarity to ore deposits, these four critical configurations are most like sandstone deposits, with the depositional agents either being reducing chemistry or sorption. The tree continues along branch "K" to potential critical configurations in the saturated zone.

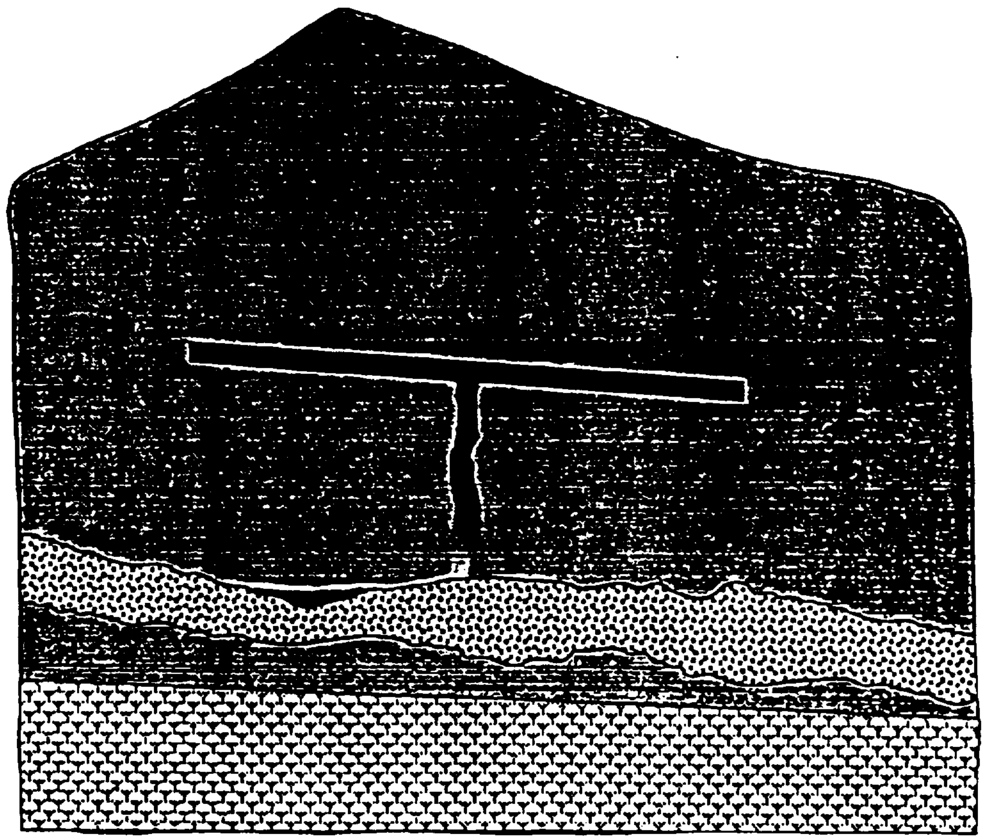

Figure 15. Illustration of critical configuration occurring in topographic lows of TSbv.

4.3.1.2 FEP-Tree Segments FF-2a – FF-2c

Tree branch "J" is similar to branch "I," except that it considers transport and concentration of colloids (Figure 16). Because of the low solubility of plutonium, this branch is expected to be the most important for the transport and re-concentration mechanisms for this nuclide. The instability, adherence, and filtration of colloids may limit the range into the far field that these processes must be considered. As is the case for solutes, separation of absorbers from fissile materials, and separation of fissile materials among themselves can occur. Potential configuration **FF-2a** results from the filtering and concentration of plutonium colloids in dead-end fractures. In the rock immediately surrounding the drifts, there may be substantial fracturing and an extensive fracture network formed by stress-relief and thermal effects. This fractured zone is expected to extend about one or two drift diameters into the country rock (Jaeger and Cook, 1979). Potential critical configuration **FF-2b** is analogous to those described previously for sorption of uranium onto clays and zeolites. Lastly, critical configuration **FF-2c** illustrates a colloid filtering mechanism that could occur in topographic lows on the upper boundary of altered TSbv. Branch "L" leads to FEPs for saturated-zone critical configurations for plutonium colloids.

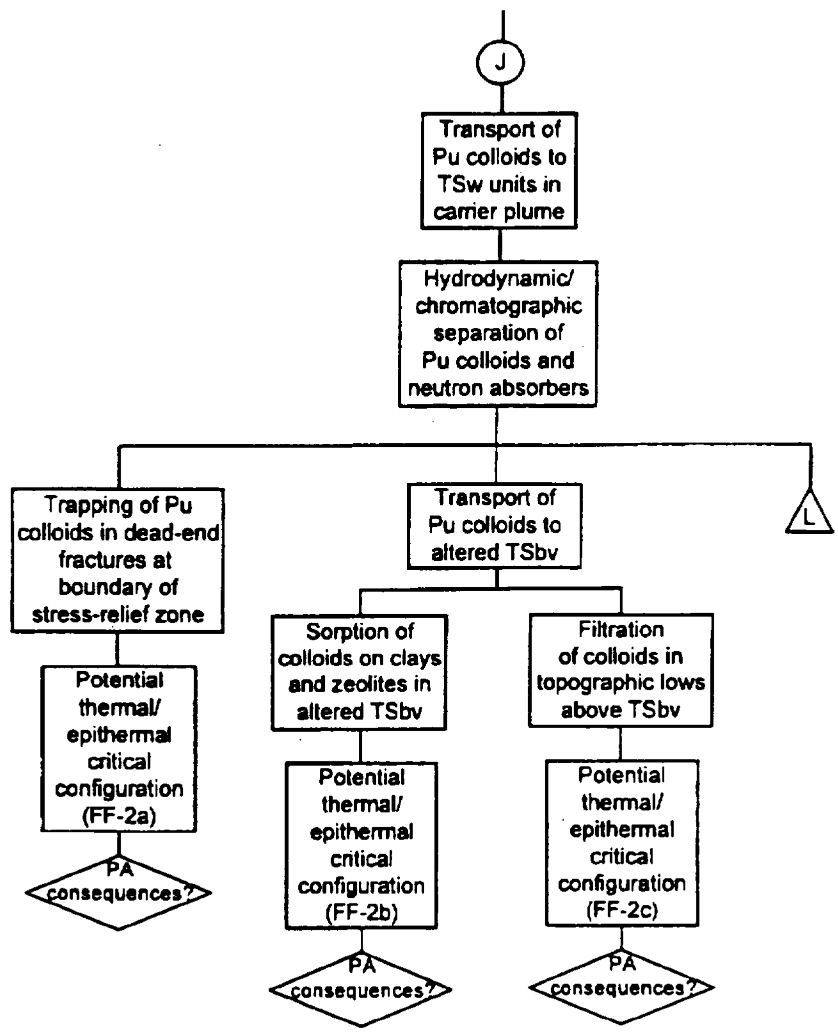

Figure 16. FEPs for far-field critical configurations for fissile colloids in the unsaturated zone.

4.3.2 Re-concentration in the Saturated Zone

Fissile materials and absorbers can be transported through the unsaturated zone to the water table and aquifers there. When contaminants reach the saturated zone, the FEP tree distinguishes between mixing of the contaminant plume with water from the tuff aquifer and no mixing. It is expected that dilution by mixing will effectively eliminate the possibility of re-concentration and development of potential critical configurations. Thus, only the "non-mixed branch" is expanded, however the other branch will be reexamined if future data suggest it is a concern.

If the source of fissile material that reaches the far field is commercial SNF, the ^{238}U that is transported with the ^{235}U will effectively prevent any criticality because of the absorption of fission neutrons by the ^{238}U. However, there is a scenario that could possibly produce criticality in the far field. If uranium is transported from the waste package and the plutonium remains behind (because of its considerably lower solubility), then the ^{239}Pu can decay to ^{235}U with a 24,100-year half life. The ^{235}U can then be transported to the far field where it can re-concentrate to form a potential critical configuration at a location other than where the ^{238}U is located. (The start of this scenario is shown in branches "D" and "E.")

The long-distance transport and potential re-concentration of colloids is not well understood, and has not been expanded in this FEP tree. However, given the very low solubility of plutonium in groundwater, colloid transport may be the only reasonable way for potential critical configurations for plutonium to occur.

4.3.2.1 FEP-Tree Segments FF-3a – FF-3e

FEP tree branch "M" (shown in Figure 17) considers potential critical configurations that occur if the uranium that arrives at the saturated zone is pure fissile material (specifically, ^{235}U). This could happen if the uranium source in the waste package was either HEU or plutonium that decayed to ^{235}U. Water upwelling along faults (e.g., the Bow Ridge fault or the Solitario Canyon fault) may have sufficiently different geochemical properties (such as system Eh or pH) that solutes in the carrier plume may precipitate in fractures. **FF-3a** considers a potential epithermal or thermal critical configuration as a result of this precipitation. Precipitation reactions can also occur if the contaminant plume mixes with waters from deeper in the tuff aquifers below the reduction front that have reducing chemistry (configuration **FF-3b**). This reaction is expected to occur at greater depths than that postulated for configuration FF-3a.

If organics are present in the aquifers (such as carboniferous deposits from detritus in alluvium, or accumulations of organics from paleo-deposits), these can provide precipitation sites where the uranium is reduced to less-soluble oxidation states. Potential configurations **FF-3c** and **FF-3d** illustrate these situations.

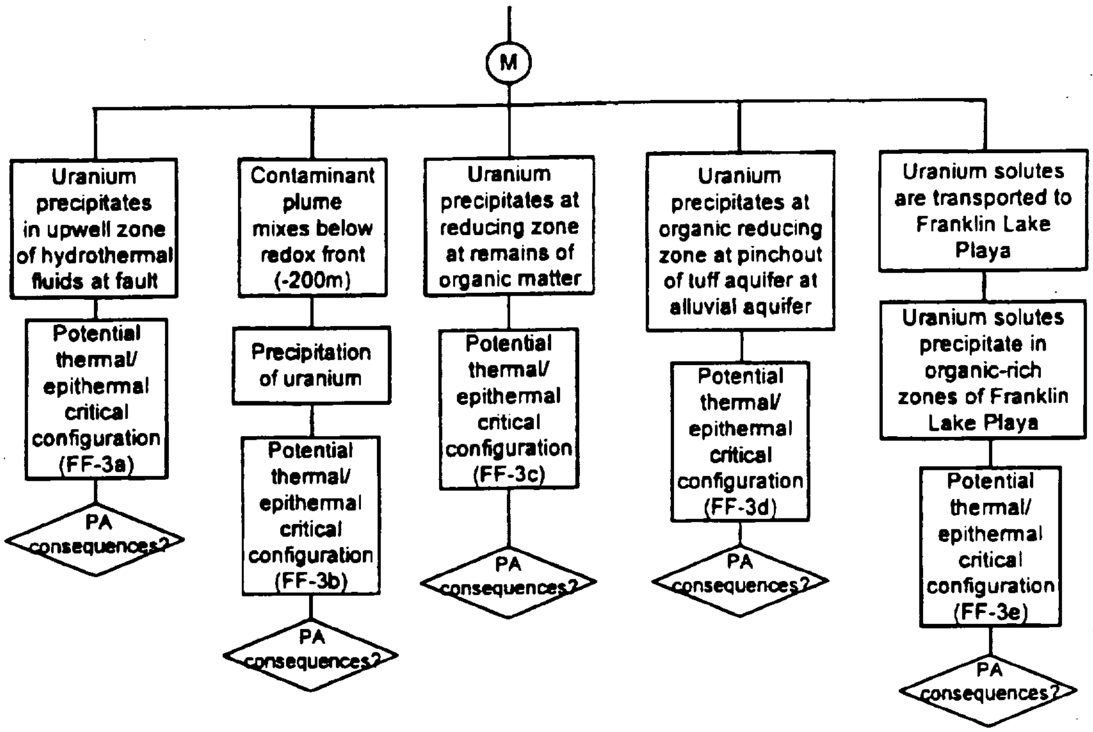

Figure 17. FEPs for far-field critical configurations for fissile solutes in the saturated zone.

Lastly, if uranium is transported unmixed to the Franklin Lake Playa or another outfall from the regional flow system, there are organic and inorganic materials associated with the lake-bed deposits there that can reduce and potentially concentrate it. Configuration **FF-3e** shows the possibility of an epithermal/thermal critical configuration where there is sufficient water. The water that transports the uranium to the point of re-concentration is likely sufficient to provide the moderator for a thermally critical configuration. Additionally, the Nevada basin and range area is known for its deposits of borates; it is therefore not unlikely that such deposits will be found at Franklin Lake Playa (van Konynenburg, private communication; Bureau of Mines, 1985). The presence of these naturally occurring absorbers must be considered when evaluating these potential critical configurations. Configuration FF-3a is similar to unconformity ore deposits; configurations FF-3b, FF-3c and FF-3d are like sandstone deposits, while FF-3e is similar to calcrete.

4.3.2.2 FEP-Tree Branch "N"

This branch considers potential criticalities that could occur for unmixed contaminant plume in which the uranium is also unseparated into enriched ^{235}U. Whether uranium and neutron absorbers separate is dependent on the nature of release of contaminants from the repository. If the release is a single event (a "slug" of contaminant) then sorption and dispersion can result in spatial and temporal separation of the uranium from absorbers. A slug release could occur from the failure of a single (or a few nearby) waste packages over a short period of time. However, widely distributed, or continuous releases from the repository may obscure the effects of separation. Most of the same processes postulated in the previous section apply for this branch also, so it is not expanded in this tree.

NEED BREACH DISCUSSION ON DIAGRAM.

5.0 SELECTION OF SCENARIOS FOR TSPA-VA

There are two factors that can make scenarios important for TSPA-VA analyses — probability of occurrence and PA consequences. As was discussed in Section 3, there is enough fissile material contained in any of the waste types to theoretically provide sufficient fissile material for nuclear criticality. Thus, there is no waste type that is "too small" an amount to be able to ignore as a potential criticality source. Although several of the in-package potential criticalities are more applicable to some types of fissile-material waste than to others, no scenarios can be automatically excluded because they are primarily relevant to an "unimportant" single waste type or waste-package construction/configuration.

All the FEPs contributing to geologic assembly of a potential critical configuration must be considered in the estimation of either relative or absolute probabilities. Because there are so many unknowns, variabilities, and uncertainties, it may not be possible to develop absolute probabilities with much confidence. However, given our knowledge of the design and engineering, it may be possible to estimate RELATIVE probabilities for some in-package configurations relative to other configurations.

- Because all the criticality scenarios require waste-package breach, any differences in waste-package construction or contents (as they affect heat output, for example) can help estimate relative probabilities.
- Given a waste-package breach, the degradation resistance of the waste form can influence the formation of a critical configuration. One method for estimating the relative probability of occurrence for a potential criticality scenario is to weight according to the fraction of the total number of waste packages containing waste of a specific type (e.g., CSNF, DOE SNF, Pu-glass, etc.).
- For in-package criticalities, it may be possible to roughly estimate relative probabilities by comparing the responses of the various waste types and waste-package internal structures to identify those combinations that are relatively more or less resistant to corrosion and degradation.

PA consequences can be estimated somewhat more directly than probabilities. An "efficient" method of evaluating the impact of a criticality event on total-system performance is to follow a three-step analysis:

- *Assume that a critical configuration exists, and calculate the impacts.* For example, assume that the contents of one waste package containing CSNF of a given burnup and age have formed a configuration with k_{eff} of 1.0. Based on the FEPs of the scenario, assume that the optimum conditions for criticality exist. For these conditions (e.g., the geometry, the amounts of fissile material, moderator, and neutron absorbers present), estimate the duration of the criticality and the number of fissions that would occur. Calculate the fission-product and actinide inventories created by the criticality to see if they represent a significant modification to the existing radionuclide inventory. One of the factors that determines whether the additional inventory is a significant perturbation depends on the time at which the criticality event occurs. If the perturbation to the inventory warrants further investigation, then do the next step.
- *Investigate the geologic processes and conditions necessary to create the critical configuration.* By modeling the processes, rates, and timings of the FEPs that must occur to create the critical configuration, additional information can be developed that may change the parameters of the criticality (such as fissile-material availability, moderator, etc.). By recalculating k_{eff}, the power and duration of the criticality, and the resulting radionuclide inventory, the significance of the criticality to repository performance (in the form of an alteration to the radionuclide inventory) can be reevaluated. Again, if the criticality appears to cause a significant perturbation to the inventory, the final step can be undertaken.
- *Perform a TSPA analysis using the modified inventory.* The radionuclide inventory becomes the source term for groundwater flow and transport analyses and dose calculations. Again, the timing of the creation of the additional source term may be a factor. Impact of the criticality on repository performance can be directly reported as an increase in dose or releases as a function of time, or other measure.

DO A CRITICALITY CALCULATION? FOR THOSE INITIALLY SCREENED AS CREDIBLE. FURTHER SCREEN TO SEE IF REL. PROB. IS LOW THAT CONDITIONS ARISE.

By using this three-step method, unnecessary analyses will not be done to investigate scenarios that have no PA impact.

5.1 Important In-Package Scenarios

Table 2 summarizes the in-package critical configurations discussed in Section 4.1. The "Relative Probability" column in Table 2 does not consider consequences of criticalities, and thus cannot be the sole discriminator of the scenarios. After first screening on relative

MOVE TO ~~END OF~~ PREVIOUS SECTION. DISCUSS HOW THOSE W/ MEDIUM OR HIGHER ARE KEPT.

probability, the consequences must be evaluated, according to the three-step method given above. The scale used for relative probabilities is as follows:

WHO DID RANKING WHERE DID THIS COME FROM

1. unlikely
2. low
3. medium
4. high
5. certain

The potential critical configurations that will be considered for inclusion in TSPA-VA are **IP-1b**, **IP-2b**, **IP-3b**, **IP-4b**, and **IP-5a**. All have "medium" relative probability of occurrence. Configuration IP-1b (degraded DOE SNF in water) is composed of enriched uranium in a homogeneous geometry with moderator. Furthermore, the aluminum-clad DOE spent fuel will be much more susceptible to corrosion than the Zircaloy-clad CSNF. The Waste-Package Development (WPD) group is currently analyzing this scenario; their results can be applied to the TSPA-VA analysis. Configuration IP-2b applies to plutonium glass/ceramic. The homogeneous mixture of plutonium and clay provides a favorable geometry for criticality. However, it requires over 50 kg of Pu in a waste package to provide enough fissile material for a criticality. An analysis of the neutronics and geochemical processes has been done by the WPD group (CRWMS M&O, 1997a); that work found that dissolution and separation of the gadolinium neutron absorber material from the waste form was possible over time periods of greater than 40,000 years. If the waste package initially contained sufficient plutonium, it and the ^{235}U daughter product could potentially go critical. Further analyses of the PA consequences for this scenarios can be based on this work using the three-step method outlined above. Configuration IP-3b is a scenario for the most common waste to be disposed of in the repository — Zircaloy-clad CSNF. Because this scenario assumes the basket only partially collapses (so that the neutron absorber is separated from the fuel, but the fuel-assembly spacers remain intact), the fuel-pin spacing is optimal for criticality. This has also been analyzed by the WPD group (CRWMS M&O, 1997f). IP-4b is similar to IP-1b, except that the hydrated aluminum and glass corrosion products are assumed to contain enough water to provide moderation. This scenario is also being analyzed by the WPD group, as is IP-1b. Lastly, configuration IP-5a is similar to IP-2b; as for configuration IP-4b, the clays are expected to provide sufficient water for moderation; The requirement for at least 50 kg of Pu in the waste package applies for this configuration also. It has been analyzed by the WPD group (CRWMS M&O, 1997a).

Although configuration IP-3c is thought to have a "high" relative probability for criticality, it is applicable only to the MPC. If the "wagon wheel" spacer for the SNF waste collapses, and the neutron absorber in the Bor-Al spacer is separated from the spent fuel, then the spent fuel can consolidate to its optimal spacing for criticality. This scenario has not been analyzed by the WPD group because the MPC is not currently an active design option. If this package is reconsidered, an analysis will be done.

The remaining configurations listed in Table 2 are considered to have "low" relative probability. Some of the reasons for the low probabilities are as follows:

IP-1a: Presence of neutron absorber should reduce reactivity to that criticality is not possible.

IP-2a: Flushing of absorbers in "bathtub" mode may be less efficient than in flow-through mode (configuration IP-2b); requires at least 50 kg of Pu in waste package.

IP-2c: Requires such rapid waste-form degradation that the ^{239}Pu does not fully decay to ^{235}U (i.e., less than 50,000 years); waste-package and waste-form design should preclude this occurrence.

IP-3a: Reduced reactivity of fuel pins when they consolidate, and presence of ^{238}U to absorb neutrons.

IP-3d: If the wagon wheel spacer does not collapse, then the fuel assemblies are not in an optimal configuration for criticality, according to waste-package design.

IP-4a: The amount of water in the corrosion products may be insufficient to provide moderation.

IP-6a: Insufficient water for moderation.

The scenarios under consideration are those thought to have relatively high probabilities of occurrence. As part of the selection process, an initial estimate of the consequences and will be made. (This is the first step in the three-step screening method listed above.) For example, if the design of the Pu-glass waste packages specifies less than 50 kg of plutonium per package, or if it is unlikely that 50 kg of Pu can be mobilized to form a critical configuration, then the PA consequences of this configuration are nil, because there is no possibility of criticality. For those scenarios that meet the first test, an analysis of the geologically driven processes will be done. An example of this is a determination of the likelihood that waste-package corrosion will cause failure at the top before failure at the bottom. (Many of the selected configurations assume a "bathtub" containing water for moderation.)

Table 2. Summary of In-Package Critical Configurations

Configuration	Waste Form	Neutron Absorber	Fuel	Failure Necessary for Criticality	Moderator/ Geometry	"Relative Probability"
IP-1a	Al-clad DOE SNF, & DHLW	Boride-loaded steel plates	HEU and MEU	Waste degradation only	Liquid water; homogeneous fuel and moderator with absorber nearby	2 – absorber should prevent criticality
IP-1b	Al-clad DOE SNF, & DHLW	Boride-loaded steel plates	HEU and MEU	Waste degradation; separation of fuel from absorber	Liquid water; homogeneous fuel and moderator	3 – fuel separated from absorber
IP-2a	Pu-glass/ ceramic	Gd, Hf, (B)	^{239}Pu	Glass degradation; acidic conditions; absorbers flushed	Water & hydrated clay; homogeneous fuel/ moderator	2 – if Pu > 50 kg; absorbers dissolved and flushed
IP-2b	Pu-glass/ ceramic	Gd, Hf, (B)	^{239}Pu	Glass degradation; WP bottom failure; acidic conditions; absorbers leached	Hydrated clays; homogeneous fuel and moderator	3 – if Pu > 50 kg; clay provides moderating water
IP-2c	Pu, U	B, Gd	^{239}Pu	Waste-form degradation in less than 50k years; absorber separation	Water and hydrated clays; homogeneous fuel and moderator	2 – rapid W. F. degradation required for there to be any Pu left
IP-3a	stainless-steel clad SNF	Boride-loaded steel plates	LEU (U & Pu)	Basket collapses, fuel assemblies consolidate; absorber mobilized	Liquid water between fuel-pin assemblies, reduced fuel-pin spacing	2 – ^{238}U, and reduced reactivity of closer pins reduces reactivity
IP-3b	Zircaloy-clad SNF	Boride-loaded steel plates	LEU (U & Pu)	Basket partially collapses; absorbers mobilized	Liquid water between fuel-pin assemblies; some absorbers remain	3 – neutron absorption by ^{238}U, FeO, and B reduces reactivity
IP-3c	CSNF	Bor-Al wagon wheel (MPC)	LEU (U & Pu)	Absorber mobilized; "wagon wheel" later collapses; fuel assemblies consolidate	Liquid water between fuel-pin assemblies, optimal fuel-pin spacing;	4 – neutron absorption by ^{238}U; optimal spacing increases reactivity
IP-3d	CSNF	Bor-Al wagon wheel (MPC)	LEU (U & Pu)	Absorber mobilized	Liquid water between fuel-pin assemblies, non-consolidated pin spacing;	2 – neutron absorption by ^{238}U; spacing decreases reactivity
IP-4a	Al-clad DOE SNF, & DHLW	Boride-loaded steel plates	HEU and MEU	Waste degradation only	Hydrated corrosion products; homogeneous fuel & moderator; absorber nearby	2 – absorber should prevent criticality; limited water
IP-4b	Al-clad DOE SNF, & DHLW	Boride-loaded steel plates	HEU and MEU	Waste degradation; separation of fuel and absorber	Hydrated corrosion products; homogeneous fuel & moderator	3 – fuel separated from absorber
IP-5a	Pu-glass/ ceramic	Gd, Hf, (B)	^{239}Pu	Glass degradation; absorbers leached through WP bottom	Hydrated clays; homogeneous fuel and moderator	3 – if Pu > 50 kg; less moderating water
IP-6a	CSNF	Bor-Al wagon wheel (MPC)	LEU (U & Pu)	Wagon wheel degrades; absorbers flushed	Intact fuel assemblies; hydrated corrosion products	1 – optimal fuel-pin spacing; limited water

5.2 *Important Near-Field Scenarios*

The near-field critical configurations from Section 4.2 are summarized Table 3. Only potential critical configuration NF-4a has a "medium" relative probability of occurrence. Based on work described in CRWMS M&O (1997g), credible geochemical concentration processes have not been identified that can cause sufficient fissile-material re-concentration to permit criticality. Thus, precipitation of uranium onto tuffs or sorption has been modeled to result in concentrations of only about 0.1%. Such concentrations are simulated only after using favorable pH and solubility parameters. These analyses have also shown that non-fissile materials also precipitate into the void spaces of the concrete or rock. These precipitates compete with the fissile-material, and can thus reduce the fissile concentration, which reduces the likelihood of these scenarios. Other factors to consider include:

NF-1a, NF-1b: It may be difficult to have acidic conditions outside the waste package sufficient to dissolve the neutron absorbers.

NF-2a: Although the clayey mass may contain significant fissile material, the planar geometry hypothesized for this configuration is unfavorable for criticality.

NF-3a – NF-3c: Filtration and deposition of non-fissile material can occur, reducing the potential for plutonium deposition; this will reduce the capacity for plutonium concentration.

NF-4a – NF-4e: Water must pond in the drift to a depth of about 1 meter to reach and corrode the underside of the waste package.

NF-4b, NF-4c: Geometry in pool disturbed by falling rock must be optimal.

Configuration NF-4a is considered the most likely of the near-field scenarios because the contents of a waste package are deposited in the drift, providing potentially sufficient fissile material to support criticality. No further re-concentration may be required to produce a critical configuration. This configuration has not yet been analyzed by the WPD group, although it is planned. This configuration can develop for any type of waste-form/waste-package combination. The scenario that will be considered for TSPA-VA uses Zircaloy-clad CSNF, since the repository is expected to contain the largest quantity of this waste type.

Table 3. Summary of Near-Field Critical Configurations

Config-uration	Fuel	Concentration Mechanism	Moderator/Geometry	"Relative Probability"
NF-1a	U	Sorption onto zeolites from altered cement, ferric oxides	Water, SiO_2; variable geometry	1 – difficult to build up large uranium concentrations
NF-1b	U	Precipitation onto tuff	Water, SiO_2; variable geometry	1 – difficult to build up large uranium concentrations
NF-2a	U, Pu	Acidic conditions leach absorbers from clayey mass	Hydrated corrosion products; planar geometry	1 – unfavorable geometry; acidic conditions unlikely
NF-3a	Pu	Filtration through corrosion products	Water, SiO_2; variable geometry	1 – co-deposition of inert materials reduces fissile concentration
NF-3b	Pu	Sorptive separation of absorbers	Water, SiO_2; variable geometry	1 – competitive sorption between fissile material and absorbers
NF-3c	Pu	Sorption onto finely divided concrete	Water, SiO_2; variable geometry	1 – competitive sorption between fissile material and absorbers
NF-4a	U, Pu	Mechanical transport from WP	Water, SiO_2; variable geometry	3 – like IP-3b, except outside of package
NF-4b	U, Pu	Stratification of FM; mixing with moderator by disturbance	Water, SiO_2; planar -> toroidal geometry	1 – geometry must change to increase reactivity
NF-4c	U, Pu	Preferential dissolution of Uranium; filtration of Pu	Water, SiO_2; variable geometry	1 – must happen soon enough that Pu has not decayed
NF-4d	Pu	Stratification of Pu; mixing with moderator by disturbance	Water, SiO_2; variable geometry	1 – geometry must change to increase reactivity
NF-4e	Pu, U	fixed Pu decays to U	Water, SiO_2; variable geometry	1 – rapid WP and WF degradation required

5.3 *Important Far-Field Scenarios*

Table 4 summarizes potential far-field critical configurations discussed in Section 4.3. None of them have a relative probability of occurrence thought to even be "medium." Most can be eliminated because of low concentrations of the fissile-material solute being transported, the displacement of fissile-material precipitation or sorption by non-fissile precipitates mentioned above, and the low chemical potentials for reduction reactions. If the hydrological conditions remain the same, epigenetic uranium ore bodies of the type potentially leading to critical configurations could form only over time periods of millions of years. Furthermore, models for colloidal transport in Yucca Mountain rock must be further developed to be able to characterize this as a mechanism for far-field re-concentration.

Specifically, there are no analyses or data to characterize the source of reducing fluids in faults or fractures called out in configuration FF-3a. Similarly, there are no identified analyses to characterize a reducing front assumed for FF-3b. As prior analyses have shown (CRWMS M&O, 1996a), a large concentration of organic matter (such as logs) is required to reduce sufficient uranium to produce a potentially critical configuration as described for FF-3c. Formation of calcrete-type deposits, as postulated in FF-3e, are unlikely because of the requirement that an oxidizable mineral co-deposit (such as vanadium) be present. Such mineralization has not been found at the Franklin Lake Playa.

Configuration **FF-3d** appears to be the only one for which credible arguments may be developed. The requirements for a large concentration of organic matter may be reduced somewhat by flow channeling in the alluvium. As an example analysis of the TSPA impacts of far-field criticality, this scenario is the most pertinent. The WPD group has not analyzed this case, although they have done a similar one.

Table 4. Summary of Far-Field Critical Configurations

Configuration	Fuel	Concentration Mechanism	Moderator/Geometry	"Relative Probability"
FF-1a	U	Precipitation from carrier plume due to pH change	Water, SiO_2; cylindrical/spherical geometry	1 – low concentration of solute; low reactive potential of country rock
FF-1b	U	Sorption onto clays and zeolites in TSbv	Water, SiO_2; variable geometry	1 – limited void space for accumulation of fissile
FF-1c	U	Accumulation in topographic lows; precipitation from chemical changes in perched water	Water, SiO_2; planar geometry	1 – low concentration of solute; low reactive potential of country rock
FF-2a	Pu	Filtration of colloids in fractures	Water, SiO_2; linear/parallel-plate geometry	1 – unlikely that significant number of colloids can travel to far field
FF-2b	Pu	Sorption onto clays and zeolites in TSbv	Water, SiO_2; variable geometry	1 – unlikely that significant number of colloids can travel to far field
FF-2c	Pu	Accumulation in topographic lows; filtration by clays	Water, SiO_2; planar geometry	1 – unlikely that significant number of colloids can travel to far field
FF-3a	U	Precipitation by reducing fluids from Pz carbonates into faults/fractures	Water, SiO_2; variable geometry	2 – no analyses or data to characterize source of reducing fluids
FF-3b	U	Precipitation by reducing front (groundwater resident in tuffs)	Water, SiO_2; variable geometry	2 – no identified analyses; may not have sufficient reducing potential
FF-3c	U	Precipitation by organic matter in alluvium	Water, SiO_2; variable geometry	2 – need large concentration of organics to occur
FF-3d	U	Precipitation by organic material in restricted aquifer	Water, SiO_2; variable geometry	2 – potentially higher concentrations by flow channeling
FF-3e	U	Precipitation by evaporation	SiO_2; variable geometry	1 – requires vanadium; evaporation will concentrate U in soluble form; presence of boron

6.0 SUMMARY

Potential critical configurations are most likely to form within degraded waste packages, primarily because of the greater amount of fissile material available. The in-package scenarios selected for consideration include almost all the waste types that contain fissile material — commercial spent nuclear fuel, DOE highly enriched spent nuclear fuel, and plutonium-loaded glass. No configurations were identified that apply specifically to the Naval SNF or MOX. Both the "bathtub" and "flow-through" waste-package failure modes are included. One waste-package design that may result in the highest probability of in-package criticality is not being investigated, because that package design is not currently under consideration for use at the potential Yucca Mountain repository. If the design is reconsidered in the future, it will be analyzed for criticality potential.

For both near-field and far-field potential critical configurations, few credible mechanisms have been identified for re-concentrating fissile material solutes or colloidal suspensions in the Yucca Mountain rock. Neither precipitation due to pH changes or reducing environments, nor sorption appear to be able to produce sufficient concentrations for criticality over the time periods of interest for repository performance. The one near-field critical configuration considered for further investigation is essentially an extension of in-package criticalities where the entire contents of a degraded waste package can be deposited in the drift.

Because of the difficulty in identifying mechanisms for fissile-material re-concentration in the unsaturated zone or the saturated zone over the time periods of interest, no far-field critical configurations were selected, based on their probability. The one configuration thought to be most credible, based on a combination of concentration effects, will be considered. This can be analyzed using step 1 of the three-step method given above to see if there are any PA consequences from the occurrence of such a far-field criticality.

7.0 REFERENCES

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Attachment
Complete FEP diagram

Part. ant M&O
Database - MOYMP
Prepared - 25-SEP-96:00:45:45

Yucca Mountain Site Characterization Project
Planning and Control System (PACS)
Participant Planning Sheet (PSA03)

Inc. Dollars in Thousands (Esc.)

P&S Account - 1.2.5.4.1 M&O

P&S Account Title - Total System Performance Assessment

PWBS Element Number - 1.2.5.4.1

PWBS Element Title - Total System Performance Assessment

Baseline Start - 01-oct-1996
Baseline Finish - 19-feb-1999

Fiscal Year Distribution

Annual Budget	Prior	FY1997	FY1998	FY1999	FY2000	FY2001	FY2002	FY2003	FY2004	FY2005	FY2006	Future	At Complete
	0	2439	3672	0	0	0	0	0	0	0	0	0	6111

Statement of Work

Perform preliminary, pre-decisional work that will allow the performing of analyses that demonstrate with reasonable assurance that the total containment system will meet the regulatory requirements. Assist in the review and further development of total system performance assessments utilizing input from waste package, site and repository performance assessment activities. Develop, verify, validate, benchmark, and document codes for assessing the performance of the repository, as needed. Identify and prioritize data required for performance assessment, utilizing appropriate uncertainty-analysis techniques. Maintain awareness of international technical advances in the area of performance assessment, and integrate into appropriate. Coordinate and manage the total system PA activity performed by subcontractors and other participant organizations. Integrate physical process submodels and data into computational models for prediction of total system postclosure performance (including uncertainties). Assess whether the Yucca Mountain MGDS will meet the overall system performance objective.

ALL DELIVERABLES ACCEPTED IAW DOE PROCEDURES FOR ACCEPTANCE REVIEWS, UNLESS OTHERWISE NOTED.

Summary Account	Title
TR541FA1	FY97 Performance Assessment Management
TR541FA2	PA Support to Follow-On Performance Confirmation
TR541FA3	PA Support to Waste Isolation Study
TR541FA4	PA Support to System Requirements Analysis
TR541FA5	PA Support to Lic. Application Plan Development
TR541FA6	PA Support to TSPA Orientation
TR541FA7	FY97 PA Interactions with NWTRB/NRC
TR541FB1	Scenarios Development for Viability Assessmen
TR541FB2	Develop TSPA-VA Methodol., Software & Assumptions
TR541FB3	TSPA-VA Chapter 8 Analyses & Documentation
TR541FB4	Abstraction/Testing of Biosphere Model
TR541FB5	Preparation of TSPA Input to NEPA
TR541FB6	PA Input to SC Semi Annual Progress Report 16
TR541FB7	PA Input to SC Semi Annual Progress Report 17
TR541FB8	Implement Process Model Changes
TR541GA1	FY98 Performance Assessment Management
TR541GA2	PA Support Follow-On Performance Confirmation
TR541GA3	PA Support TSPA-VA/PR Letter Report Preparation
TR541GA4	PA Support Final Peer Review
TR541GA5	PA Support Scenario Review/Peer Review Report
TR541GA6	PA Support Abstraction Models Review/Peer Rvw Rpt
TR541GA7	FY98 PA Interactions with NWTRB/NRC
TR541GB1	PA Input to SC Semi Annual PR18
TR541GB2	PA Input to SC Semi Annual PR19
TR541GB3	Scenarios Development of LA

TR541 Total System Performance Assessment (continued)

DELIVERABLES

Deliv ID	Description/Completion Criteria	Due Date
SL105AM3	Compl. Criticality Scenario for VA Documentation Criteria - Using information from the site, groundwater flow and transport, and near-field geochemistry activities, and other information sources (such as the Disposal Criticality Analysis Methodology Technical Report) as input, identify the features, events, and processes (FEPs) in the geohydrological and geochemical system that can lead to nuclear criticality excursions. These FEPs will include the regions in which criticality events can occur, and the criticality-control methods. FEPs are then synthesized and assembled into logical sequences to create scenarios. As appropriate, include technical information obtained from experts in fields such as nuclear criticality, geochemistry, and geohydrology in the definition of scenarios. Document the selection process of those scenarios that are thought to have the highest consequence and/or highest probability of occurrence as those to be included in TSPA-VA and on which to focus further PA analyses. Document the scenario development and selection process in a YMP report.	30-sep-1997
SL230SM3	Biosphere Mdl Abstr./Test Wkshop Results Doc. Criteria - This document will include a discussion of the context for use of the biosphere model within the YMP PA program and the goals of this Summary Account activity. Results from the workshop will include: discussion of relevant assumptions, the general approac to model abstraction and testing, the form of the product of the abstraction process, comparison to current or previous PA modeling, a review of the processes to be considered, key issues to be addressed in the abstraction process, discussion of issue that will not be addressed or may not be resolved in the abstraction process and possible implications. In addition, a schedule for completion of the abstraction/testing activity and identification of important interfaces to other areas of the program will be included. Portions of this document ~~should~~ will be suitable as an initial draft of introductory sections of the final product of this activity (due following completion of the Summary Account activity in FY 1998 and to form a chapter of the TSPA-VA document). This document shall be submitted to affected M&O organization for informal/informational review prior to delivery to YMSCO.	15-aug-1997 [illegible] 9-25-96 RAK 9/... DAY 9-25-96
SL230B1D	Document TSPA-VA Methodology & Assumptions Criteria - This deliverable will serve as the draft Introduction to the TSPA-VA document (i..e, the Introduction to the PISA Chapter 8). Th document will include a discussion of the approach to be taken in the TSPA-VA, the major assumptions to be adopted in the TSPA-VA, a detailed description of the software to be used in the TSPA-VA, appropriate verification tests of the software to be used (which may consist of comparison to process model results or analytical solutions). In addition to discussing the features events and processes (FEPs) which will be evaluated in the TSPA-VA, the document will address the rationale for not addressing certain FEPs or the effects of certain FEPs. The document will be reviewed by affected M&O organizations. This document will outline the basis for all assumptions to be evaluated in TSPA-VA. It also serves to identify the "base case" conceptual model an parameter distributions expected to used in the TSPA-VA (which might change as the TSPA analyses themsellves are conducted in FY 98). as well as the primary issues to be evaluated in the sensitivity analyses. The document will discuss the abstraction process for all the relevant process models, including: 1. UZ hydrology 2. SZ hydrology 3. UZ and SZ transport 4. Thermal hydrology 5. Near field environments 6. Waste package degradation 7. Waste form degradation 8. Radionuclide mobilization 9. Biosphere	13-aug-1997

TR541 Total System Performance Assessment (continued)

Approvals

9-25-96

Jean L Younker	9-25-96	Stephen J. Brocoum	9/25/96	Richard A. Kettell	9/25/96
Preparer - print name	Date	Technical Reviewer - print name	Date	QA Reviewer - print name	Date
Jean L Younker		Stephen Brocoum		Richard Kettell	
Preparer - signature		Technical Reviewer - signature		QA Reviewer - signature	

Pa… …pant USGS
Data… - USGSYMP
Prepared - 24-SEP-96:22:05:23

Yucca Mountain S… …aracterization Project
Planning and Control System (PACS)
Participant Planning Sheet (PSA03)

Page - 1
Inc. Dollars in Thousands (Esc.)

P&S Account - 1.2.5.4.1 USGS

P&S Account Title - Total System Performance Assessment

PWBS Element Number - 1.2.5.4.1

PWBS Element Title - Total System Performance Assessment

Baseline Start - 31-oct-1996
Baseline Finish - 29-apr-1998

Fiscal Year Distribution

	Prior	FY1997	FY1998	FY1999	FY2000	FY2001	FY2002	FY2003	FY2004	FY2005	FY2006	Future	At Complete
Annual Budget	0	50	50	0	0	0	0	0	0	0	0	0	100

Statement of Work

Provide input to support total system performance assessment activities.

Summary Account	Title
OG541FA2	Viability Assessment Scenarios Development

DELIVERABLES

Deliv ID	Description/Completion Criteria	Due Date

9/26/96

Approvals

Robert W. Craig	9/26/96	Stephan J. Brocoum	9/26/96	Richard A. Kettell	9/26/96
Preparer - print name	Date	Technical Reviewer - print name	Date	QA Reviewer - print name	Date
Debra L Edwards for Robert W. Craig					
Preparer - signature		Technical Reviewer - signature		QA Reviewer - signature	