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COMPONENTS OF AN OVERALL LICENSING  
ASSESSMENT METHODOLOGY

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## 1. INTRODUCTION AND BACKGROUND

The Nuclear Regulatory Commission (NRC), under their broad grant of authority under the Atomic Energy Act (1954), is responsible for regulating the peaceful uses of nuclear energy and regulating the radiological health and safety of the public. To implement this authority with respect to the disposal of high-level waste (HLW) and spent nuclear fuel, the NRC has promulgated technical criteria under 10 CFR Part 60. In addition, the NRC is implementing agency for the Environmental Protection Agency's (EPA) radioactive waste standards 40 CFR Part 191. The Department of Energy (DOE) is responsible for the design, construction, operation, and decommission of a geologic repository for the disposal of spent nuclear fuel and HLW. This work includes site characterization and demonstrating compliance with the appropriate regulations. In order to show compliance, the DOE is required to develop and implement a comprehensive site-assessment methodology in order to prepare a license application for the NRC. The NRC is then required to evaluate the DOE's license application. To facilitate this effort, the NRC is developing a licensing-assessment methodology. The purpose of this document is to identify the components of a licensing-assessment methodology, the processes expected to occur in the repository and its surrounding environment, their related parameters, a strategy for determining which components and parameters are the most important in the overall methodology, and a means to track the components and parameters. This report provides this information for the part of the licensing-assessment methodology that deals with the time period after the closure of the repository.

The development of any licensing-assessment methodology must be based on the

appropriate regulatory requirements. With respect to post-closure performance, these requirements are contained in the NRC's 10 CFR Part 60.113 and the EPA's 40 CFR Parts 191.13, 191.15, and 191.16. In all, there are six specific requirements, three in 10 CFR Part 60 and the three in EPA's 40 CFR Part 191 that are addressed in this document. The following sections contain descriptions of these requirements, the physical processes that need to be considered in assessing compliance with the requirements, and related phenomena and parameters. The final section of this report describes an overall methodology that could be used in assessing compliance with the requirements and a scheme for tracking the status of the relevant computer codes and parameters.

## 2. ASSESSING COMPLIANCE WITH THE REGULATIONS

The following sections discuss the processes, phenomena, and parameters that relate to demonstrating compliance with the NRC's 10 CFR Part 60 and EPA's 40 CFR Part 191 requirements. The determination of which processes and phenomena are relevant was obtained directly from the regulations wherever possible. In addition, information from Generic Technical Positions (GTPs) and Site Technical Positions (STPs) issued by the NRC were also used. Other GTPs and STPs are anticipated prior to the submittal of a license application which would also aid in identifying important processes and phenomena.

## 2.1. NRC (10 CFR Part 60.113)

The NRC regulations are designed to help meet generally applicable environment standards established by the EPA. Section 60.21 (content of application) of 10 CFR Part 60 states the NRC's expectations with respect to the contents of the license application to be submitted by the DOE. The license application should consist of general information and a Safety Analysis Report (SAR). In particular, 10 CFR Part 60.21(c)(1)(ii) outlines the type of assessments to be included in the SAR. Attention is drawn here to an important aspect of the assessments; namely, 10 CFR Part 60.21(c)(1)(ii)(C) which states:

*An evaluation of the performance of the proposed geologic repository for the period after permanent closure, assuming anticipated processes and events, giving the rates and quantities of releases of radionuclides to the accessible environment as a function of time; and a similar evaluation which assumes the occurrence of unanticipated processes and events.*

In addition to the general requirement of meeting the overall system performance objective for the geologic repository after permanent closure, the NRC rule sets out performance objectives and technical criteria for the primary components of the repository system. Section 60.113 of 10 CFR Part 60 outlines the performance objectives for particular barriers after permanent closure. Specifically, performance requirements for the "engineered barrier system" (EBS) and the "geologic setting" are stated. The EBS requirement is subdivided into two quantitative criteria pertaining to

containment within the waste packages and controlled release from the EBS boundary.

#### 2.1.1. Waste Package (10 CFR Part 60.113(a)(1)(A))

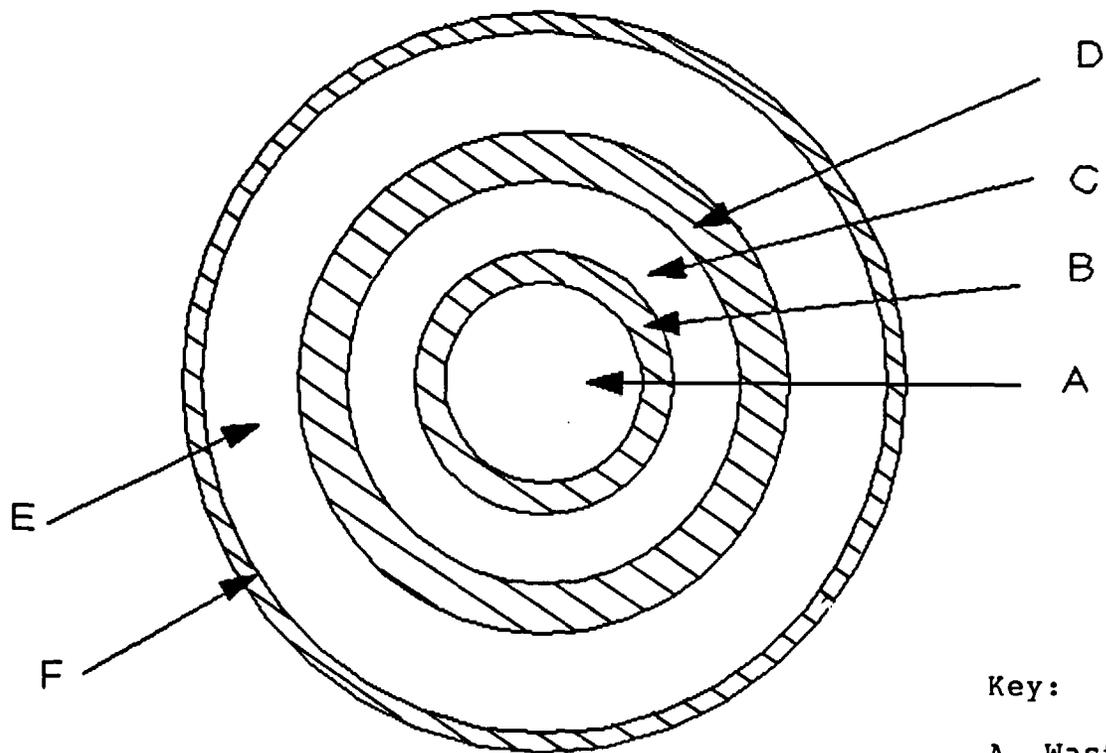
The first of the two EBS requirements is related to Waste Package Performance. The criterion states, in part, that: "Containment of HLW within the waste packages will be substantially complete for a period .... provided that such period shall not be less than 300 years nor more than 1,000 years after permanent closure of the geologic repository;" (60.113(a)(1)(ii)(A))

Placing an upper limit of 1,000-yr period on the waste package containment is not intended to restrict the container design life to a shorter period. Instead, the limit emphasizes NRC's position of not allowing credit for containment by the Waste Package component beyond that period. This is consistent with the multiple-barrier concept of not placing undue reliance on any one barrier.

##### 2.1.1.1. Definition/Description

The 10 CFR Part 60 Rule defines the waste package as meaning "the waste form and any containers, shielding, packing and other absorbent materials immediately surrounding an individual waste container." In effect, it consists of all the components placed inside the emplacement borehole in a repository. The diagram in Figure 2.1 illustrates conceptually the various components that constitute a waste package. Not every component shown in

WASTE PACKAGE COMPONENTS (Conceptual)



\*These components may or may not exist in a given design

Key:

- A- Waste Form
- B- Canister\*
- C- Crushed Rock\*/Inert Mat'l
- D- Metal Container
- E- Packing
- F- Shell\*

Figure 2.1 Components of a Waste Package

Figure 2.1 is an integral part of the waste package. Depending on the waste form and the site-specific design concept, certain components such as the canister and shell could be excluded. In general, a canister is envisioned for the reprocessed-glass waste form but not for the spent-fuel waste form. Also, the hypothetical center lines of the various cylindrical components may or may not coincide. These variations are illustrated in Figures 2.2 and 2.3, which are adapted from the Basalt Waste Isolation Project (BWIP) waste package conceptual design (Rockwell Hanford Operations, 1987). A longitudinal cross-section of the BWIP conceptual design for the HLW (reprocessed) waste form is shown in Figure 2.2 along with the terminology for various components. In this design, both a canister and a container are included. A cross-section of the BWIP conceptual design for the spent fuel (intact assemblies) waste form is presented in Figure 2.3. As may be seen the geometric centers of the different circles (i.e., components) do not coincide in this conceptual design. Also, in this design there is no canister (i.e., only a container). The gap between the waste form and inside walls of the Container is shown to be filled with crushed rock; a different design might have an inert gas or air in the gap. An important point to recognize is that the containment criterion could be satisfied even if the container fails before 300 years provided that the packing provides sufficient delay in the transport of radionuclides to the waste package surface. On the other hand, the DOE may choose to equate the waste package "lifetime" with the container lifetime in interpreting the containment requirement. Likewise, the DOE may design the waste package such that the controlled release-rate criterion is satisfied at the waste package boundary instead of at the EBS boundary. Such a design would reflect additional conservatism as far as the regulations are concerned.

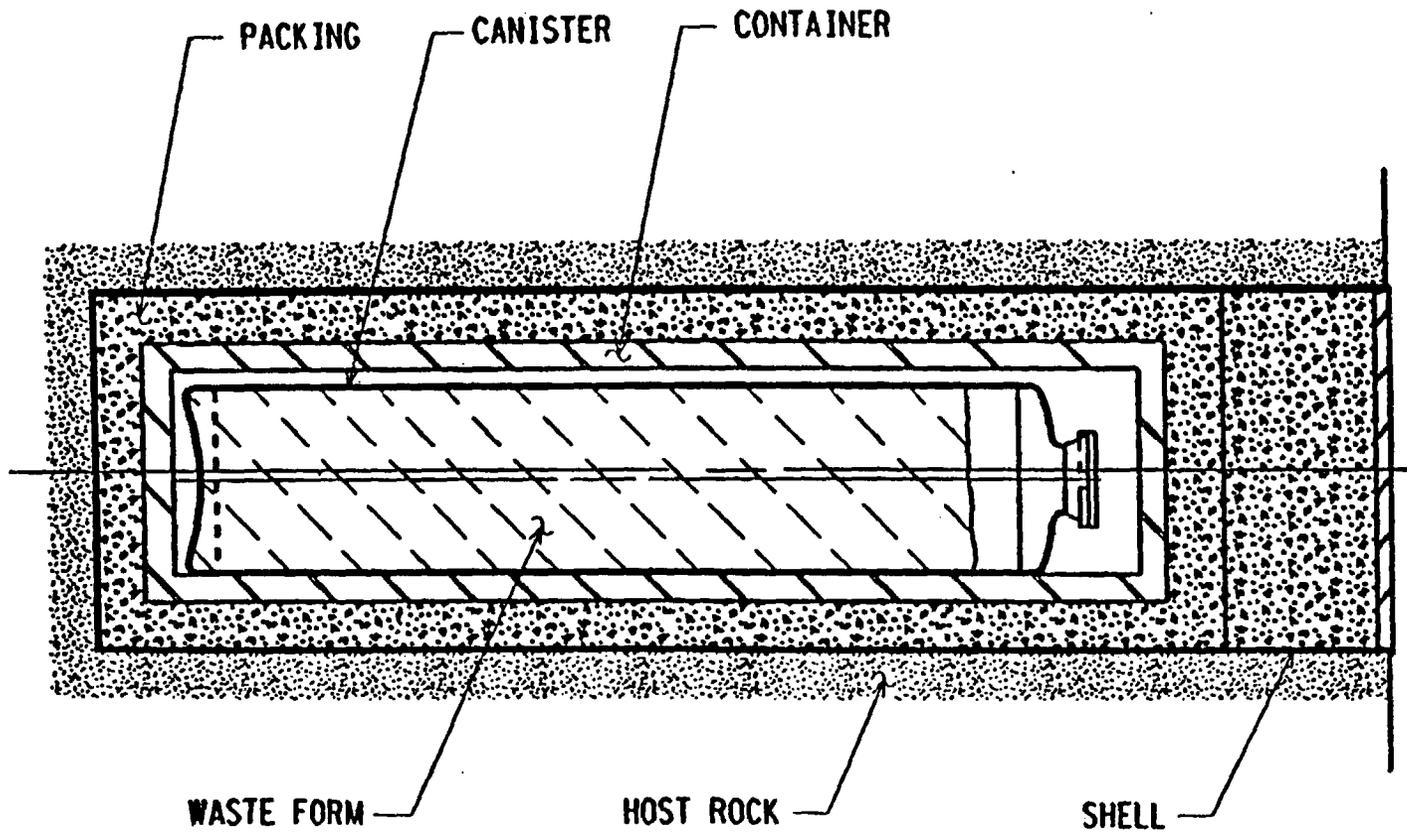


FIGURE 2.2 Diagram Illustrating Waste Package Terminology.

(Reproduced from SD-BWI-CDR-005 Document, Rockwell Hanford Operations, April, 1987)

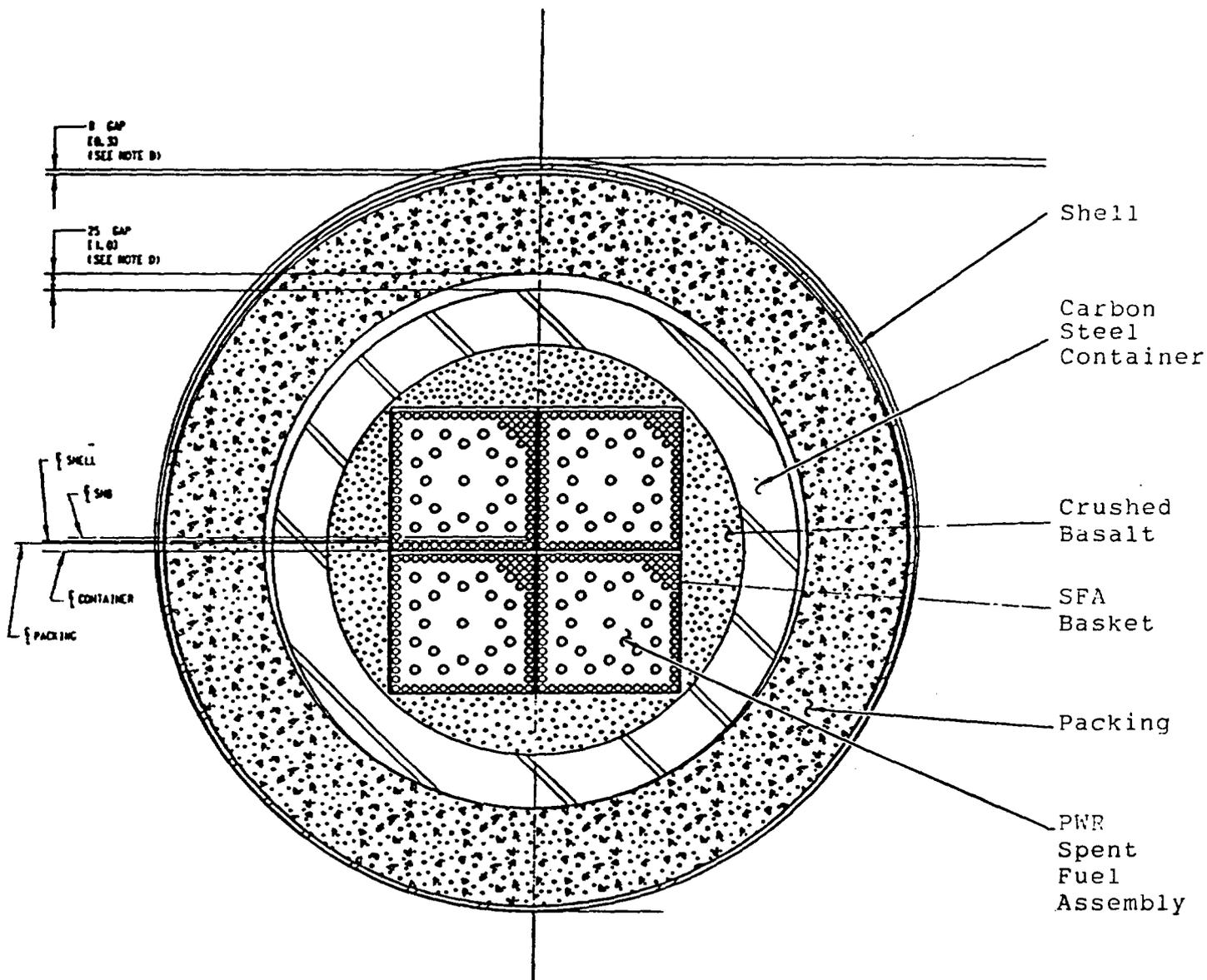


Figure 2.3 BWIP Spent Fuel Waste Package Conceptual Design

(Adapted from SD-BWI-CDR-005 Document, Rockwell Hanford Operations, April, 1987)

#### 2.1.1.2. Processes That Affect Performance of Waste Package

The performance of a waste package can potentially be affected by thermal, mechanical, transport, hydrological, and (geo)chemical processes. Certain disruptive scenarios can be postulated under which tectonic or geologic processes could lead to a premature failure of the waste package. For instance, movement along a fault or shear zone could result in breaching of one or more containers. Such effects could alternatively be considered as mechanical processes triggered by geologic processes. Other disruptive scenarios, such as drilling directly into a waste package, could occur that would breach the container and expose the waste form to the ground water.

Each of the processes identified above has specific sub-processes or phenomena that need to be considered when evaluating waste package performance. In addition, potential couplings between (or among) processes should be recognized and addressed. The processes identified earlier and their potential couplings are illustrated in Figure 2.4.

#### 2.1.1.3 Relevant Phenomena and Parameters

Many phenomena may be interrelated with couplings being weak or strong depending on the environment, and the response and time-domain of interest. Many, if not all, properties will be temperature dependent. Correlations between properties are conceivable as are non-linearities with respect to pressure and saturation.

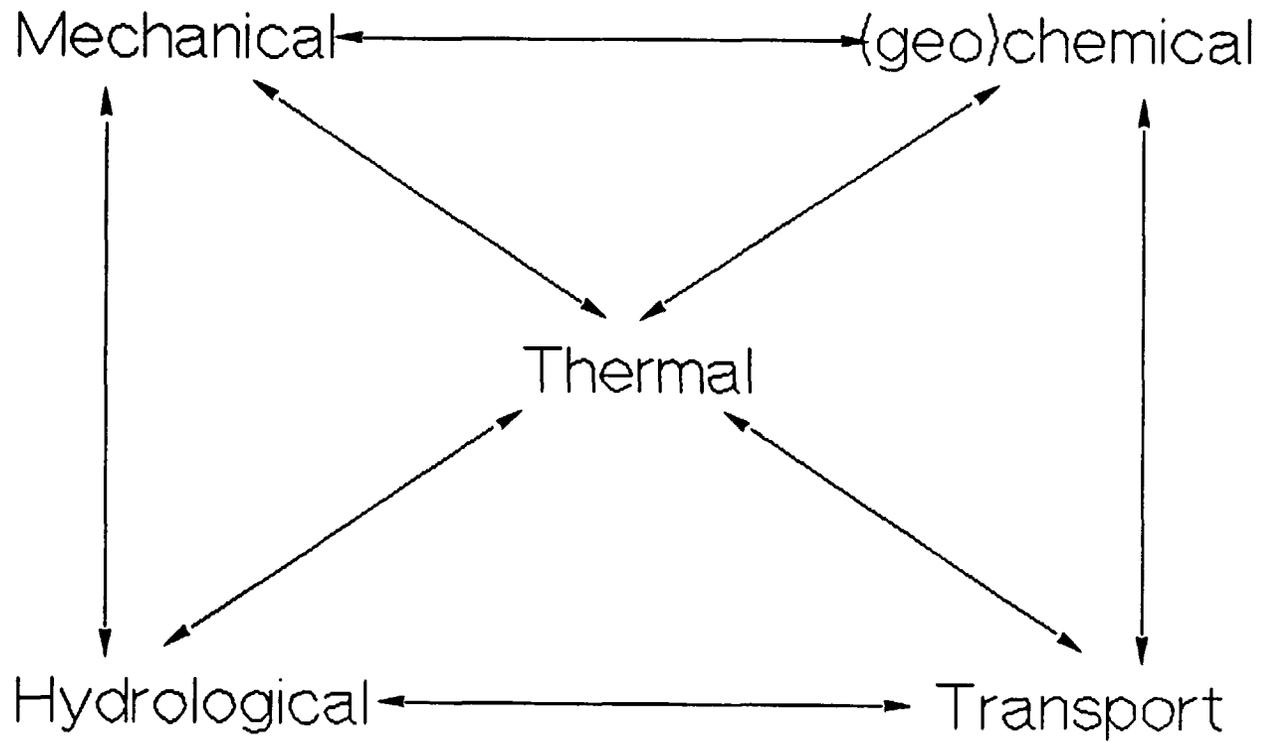


Figure 2.4 Processes and Their Potential Couplings

Thermal Processes. The phenomena under the broad category of thermal processes that need to be understood and quantified in order to characterize the waste package behavior are illustrated in Figure 2.5. Heat transfer from the waste form to the container will either be by conduction or by a combination of radiation and conduction, depending on whether the waste form is in direct contact with the container wall. Likewise, heat transfer between the container and packing (if present) will occur by conduction or by a combination of radiation and conduction. If ground water penetrates the packing, additional heat transfer within the packing may occur by convection.

The thermal properties that govern heat conduction are thermal conductivity ( $k$ ) and specific heat ( $C_p$ ). A related property is thermal diffusivity defined as the ratio of  $k$  and the volumetric heat capacity; where the volumetric heat capacity is the product of mass density and specific heat.

Thermal radiation between surfaces (e.g., between fuel assembly and container wall) occurs in proportion to the difference between the absolute temperatures raised to the fourth power. The "geometric view factor" and emissivity (both less than or equal to unity) are the properties (or parameters) governing heat transfer by radiation. In most cases, these parameters have to be determined empirically. If a filler material is used inside the container, thermal radiation may not be significant.

Heat transfer by convection can occur if fluid (or air) flows through or past the waste package at sufficiently high rates. The amount of heat transfer by convection is proportional to the temperature difference between the waste

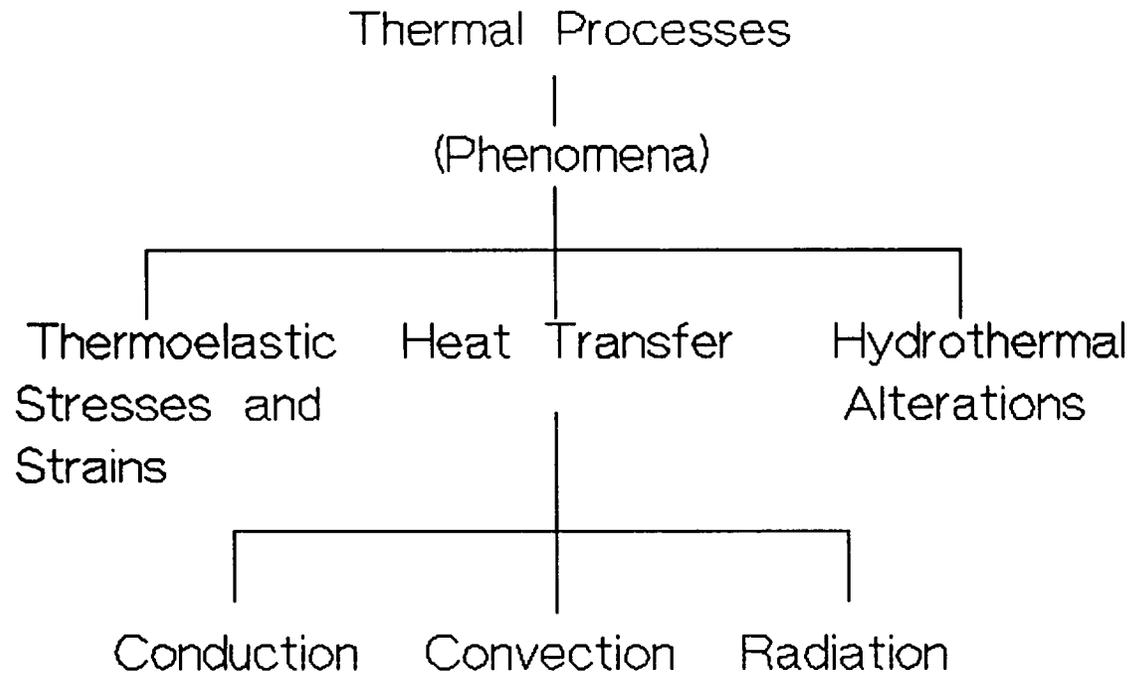


Figure 2.5 Phenomena Associated with Thermal Processes in the Waste Package

package surface and ambient temperature of the fluid. The coefficient of proportionality, known as convective heat transfer coefficient, is generally determined experimentally or empirically.

Mechanical Processes. Phenomena associated with mechanical processes that can impact the waste package performance are the thermomechanical deformation and structural (or material) failure. Several types of failure can occur: plastic yielding, brittle fracture, elastic or plastic buckling of the container, and localized failure due to stress concentration at pitting corrosion sites. Stresses in the waste package components are expected to vary with time. If resaturation occurs, the hydrostatic pressure of the ground water will be imposed as an external load on the container. In a rock that exhibits time-dependent deformation response (e.g., creep in salt), this external load might be the lithostatic pressure. Thermal stresses will change with changes in temperature and with the magnitude of temperature gradient. Thermal stresses are additive to lithostatic and excavation stresses. The container thickness is expected to decrease with time as a result of uniform corrosion; different types of corrosion are discussed later in this section. For a given external load on the container, the resultant maximum stresses within a thinner container are higher, thus making the container more susceptible to failure.

Thermal stresses are expected to develop in the waste package components. Depending on the temperature gradient in a given component, the geometry and boundary conditions, and the thermomechanical properties, these stresses may be significant. Likewise, the deformation caused by thermal expansion (or by

contraction upon cooling) could affect the integrity or containment capability of the waste package components. Thermal and mechanical properties of the waste-package components that quantify the thermoelastic stress/strain response are the coefficient of expansion and elastic moduli (e.g., Young's modulus and Poisson's ratio). In addition, mechanical strength properties of the waste-package components (yield strength, tensile and compressive strengths) will determine whether and what kind of failure might occur as a result of thermal loading.

Hydrothermal alterations, particularly in the packing material, could occur and adversely affect the waste package performance. Irreversible changes in the chemical make up, mechanical properties, and structure due to heating and subsequent cooling could degrade the initial buffering capacity and/or flow resistance of the packing material. Thermal stability, mineral composition, hydration/dehydration characteristics, and bonding between primary constituents of the packing mixture are the parameters of concern.

Radionuclide Transport Through Packing The primary mechanisms of radionuclide transport through the waste package are convection, via water, and diffusion or dispersion. For the purposes of discussing radionuclide transport and heat transfer in the waste package, any absorbent material between the container and the outer boundary of the waste package will herein be termed packing. The outer boundary of the waste package, as defined here, is the interface between the host rock and the outermost component of the emplaced waste package. Consequently, assessment of the waste package lifetime may take into consideration the travel time of the radionuclides

through any packing that is designated as part of the waste package. The rate of radionuclide migration through the packing will depend on the degree of radionuclide retardation, which is a function of the properties of the radionuclides themselves, the physical properties of the packing material, and the geochemical properties (as discussed later in this section) of both the packing and any water flowing through the packing. Physical retardation occurs primarily through the processes of diffusion into or out of adjacent flow paths under concentration gradients, diffusion into the porous matrix of the host rock, and diffusion into fluid that is not part of the bulk flow of the ground water (OECD, 1984). The physical properties of the packing which will affect radionuclide transport are: on a small scale, the pore characteristics, such as the effective porosity and the presence of closed-end pores, fracture characteristics, and tortuosity; and, on a larger scale, the dimensions of the various layers, as well as the amount of void space in the packing. Also to be considered in determining radionuclide transport and retardation are the waste inventory at a given time, the decay rates (half-lives) and decay chains of the radionuclides, the diffusion coefficients of the radionuclide species, the leach rates and solubility limits of the radionuclides, the density of the water, and the mode and time of container failure. Other parameters that will affect the process of radionuclide migration include the degree of saturation of and rate of water flow through the packing materials, since radionuclide transport is strongly coupled to water flow.

The heat generated by the nuclear waste emplaced in the repository can adversely affect the performance of the waste package. The high temperatures may alter the physical and chemical ability of the waste package packing

materials not only to retard radionuclides, but also to inhibit the infiltration of water, thus decreasing the expected containment time (i.e., lifetime) of the waste package.

In order to describe the transient thermal response resulting from the heat generated in the waste package, the various modes of heat transfer (conduction, convection, or radiation) should be considered. The amount of heat generated by the waste must also be known. The type of waste (commercial high level waste, (CHLW), defense high level waste, (DHLW), spent fuel (SF), or transuranic waste (TRU) and its initial thermal power will determine the thermal source term. The geometry, dimensions, boundary conditions, and thermal properties (discussed earlier) of the components of the waste package will dictate the transfer of heat from the source (waste form) to the waste package boundary. The presence of steam in the waste package may complicate matters, because it may transport heat convectively and may also act as an insulator because of its low thermal conductivity. Once the transient temperature response has been estimated, it can be used in the transport calculations so that the effects of heat on radionuclide transport, which are much greater than the effects of radionuclide transport on heat transfer, will be accounted for. In other words, the temperature dependence of the physical and chemical properties of the packing materials that govern radionuclide transport and of the radionuclides themselves needs to be established. For some of these properties, the dependence on temperature can be measured in the laboratory or in the field; for others, their temperature dependence will have to be assumed or derived.

The elevated temperatures also may affect the geochemistry of the packing

materials, altering their ability to chemically retard the radionuclides. To assess these effects of heat on the geochemistry, the initial geochemistry of the packing materials should be known. How these geochemical parameters may be altered at elevated temperatures should also be estimated. The relevant geochemical properties are presented below.

In addition, the high temperature may result not only in the generation of steam or in dehydration, but also in the vaporization of some of the radionuclides. This vapor phase should be taken into consideration when determining possible radionuclide migration fluxes, when calculating radionuclide transport.

Finally, to assess the effects of heat on the corrosion processes, the temperature dependence of the rates of these processes and the effects of heat on the oxidation potential of the environment surrounding the canister should also be estimated.

Geochemical Processes If there is water present in the repository, corrosion is expected to be the major failure mode of the canister and/or container. The corrosion process is strongly dependent on the geochemistry of the surrounding region. In order to assess the effects of corrosion on the lifetime of the container, it is necessary to know which types of corrosion will dominate, and what the rates of these processes will be. The types of corrosion that could occur include general (uniform) corrosion, pitting corrosion, crevice corrosion, stress corrosion cracking, hydrogen embrittlement, and microbial corrosion (Stahl and Miller, 1986). The

elevated temperatures may also affect the rate of corrosion of the container, either by increasing or decreasing the rates of the various corrosion reactions or by changing the environment (geochemistry) surrounding the container. Formation of a protective layer at temperatures above 125 C has been assumed in some BWIP analyses. (Rockwell Hanford Operations, 1987).

One approach to providing compliance with the waste package containment requirement is to use a corrosion-resistant material, such as Titanium Grade 12 or HASTELLOY Alloy C-276. (HASTELLOY is a registered trademark of the Cabot Corporation.) These materials are resistant to general corrosion, but may be susceptible to localized forms of corrosion, such as pitting, stress corrosion cracking, crevice corrosion, and hydrogen embrittlement. Another approach to providing compliance is to use a thicker steel container for which a better corrosion data base is available. However, some types of steel are also susceptible to localized corrosion under certain environmental conditions (Beavers and others, 1987). Depending on the environment, some types of corrosion may proceed much faster than others. Therefore, it is important to initially consider all types of corrosion when assessing the performance of the waste package.

The parameters that control these corrosion processes include how much water is present at the container wall, the water's redox potential (Eh) and pH, the temperature, the availability of air and hydrogen, the stresses exerted on the container, and the composition of the container. Also important are which chemical species are present in the rock, the water, and the packing material, the form in which they exist, their abundance, and the rates and equilibrium states of the various corrosion processes. In addition,

radiolysis, a process whereby the radiation from the waste alters the environment surrounding the container in such a way that corrosion rates are significantly enhanced, should also be accounted for. An additional issue to consider is the presence of water vapor and its effects, if any, on the corrosion processes.

The previous discussion on corrosion dealt with the container. However, if in the design of a particular waste package the corrosion of the canister or cladding is important, this discussion should be extended to include the canister or the cladding.

If crushed rock is used as a packing material, its ability to retard, geochemically, radionuclide transport should be estimated. It is necessary to know the extent to which chemical retardation processes such as radionuclide adsorption and desorption, colloid formation, ion exchange with naturally occurring species, stable isotope exchange with radionuclides, and chemical dissolution or precipitation of a solid phase will occur in the packing material. The parameters that are important to these processes include the specific reactions that can occur, the rates and equilibrium states of these reactions, the concentrations of the reactant species in the rock and water, the concentrations of the radionuclide species present, the concentrations of other chemical species present in the rock, and solubility limits of the radionuclides given the concentrations of these chemical species. The adsorption/desorption behavior of the packing and the various radionuclides, the pH, temperature, and pressure are also important.

The geochemistry of the packing may also affect the rate of radionuclide

release from the waste package. The rate at which radionuclides are leached from the waste form may exceed the rate at which they can be dissolved into the surrounding water, so that the radionuclides are released from the waste form but are not immediately dissolved and transported to the outer boundary of the waste package. Thus, the solubility limits of the radionuclides, which are temperature-dependent, may be important in assessing the containment by the waste package.

#### 2.1.2. Release Rates from Engineered Barrier System

(10 CFR Part 60.113(a)(1)(B))

Of the two engineered barrier system (EBS) criteria pertaining to (1) containment within the waste packages, and (2) controlled release from the EBS boundary, the first one has been addressed in Section 2.1.1. The second criterion states, in part, that:

*The release rate of any radionuclide from the engineered barrier system following the containment period shall not exceed one part in 100,000 per year of the inventory of that radionuclide calculated to be present at 1,000 years following permanent closure,....* (10 CFR Part 60.113(a)(1)(ii)(B))

By satisfying the radionuclide release rate limits at the EBS boundary, the repository system would have available only the radionuclide inventories that are limited by a known upper bound on the source term. In this manner the EBS helps control the release of radioactive material to the geologic

setting. In conjunction with the delay provided by the GWT requirement, the cumulative releases at the accessible environment over 10,000 years would then be bounded.

#### 2.1.2.1. Definition/Description

The 10 CFR Part 60 Rule defines engineered barrier system as meaning the waste packages and the underground facility. A definition of waste package has been given in Section 2.1.1. The underground facility means the underground structure (network of excavations) including openings and backfill materials but excluding shafts, boreholes, and their seals. It is important to realize that there is a distinction between the EBS boundary and the disturbed zone. Generally speaking, the disturbed zone would encompass a larger volume of the rock mass than does the EBS. In the draft GTP concerning the extent of the disturbed zone, NRC (1986) suggest that a distance of 50m from the underground openings (i.e., EBS boundary) would be reasonably conservative for defining the extent of the mechanically-disturbed zone. For the purpose of analysis, the transport of radionuclides from the EBS to the edge of the disturbed zone should be assumed to occur instantaneously. Such an assumption produces two desirable effects: (1) The analysis is simplified because the need to estimate flow and transport through the disturbed zone is eliminated and (2) additional conservatism is provided because the 1,000 year GWT requirement applies to the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment.

Illustrated in Figure 2.6 are the boundaries of the waste package, EBS and

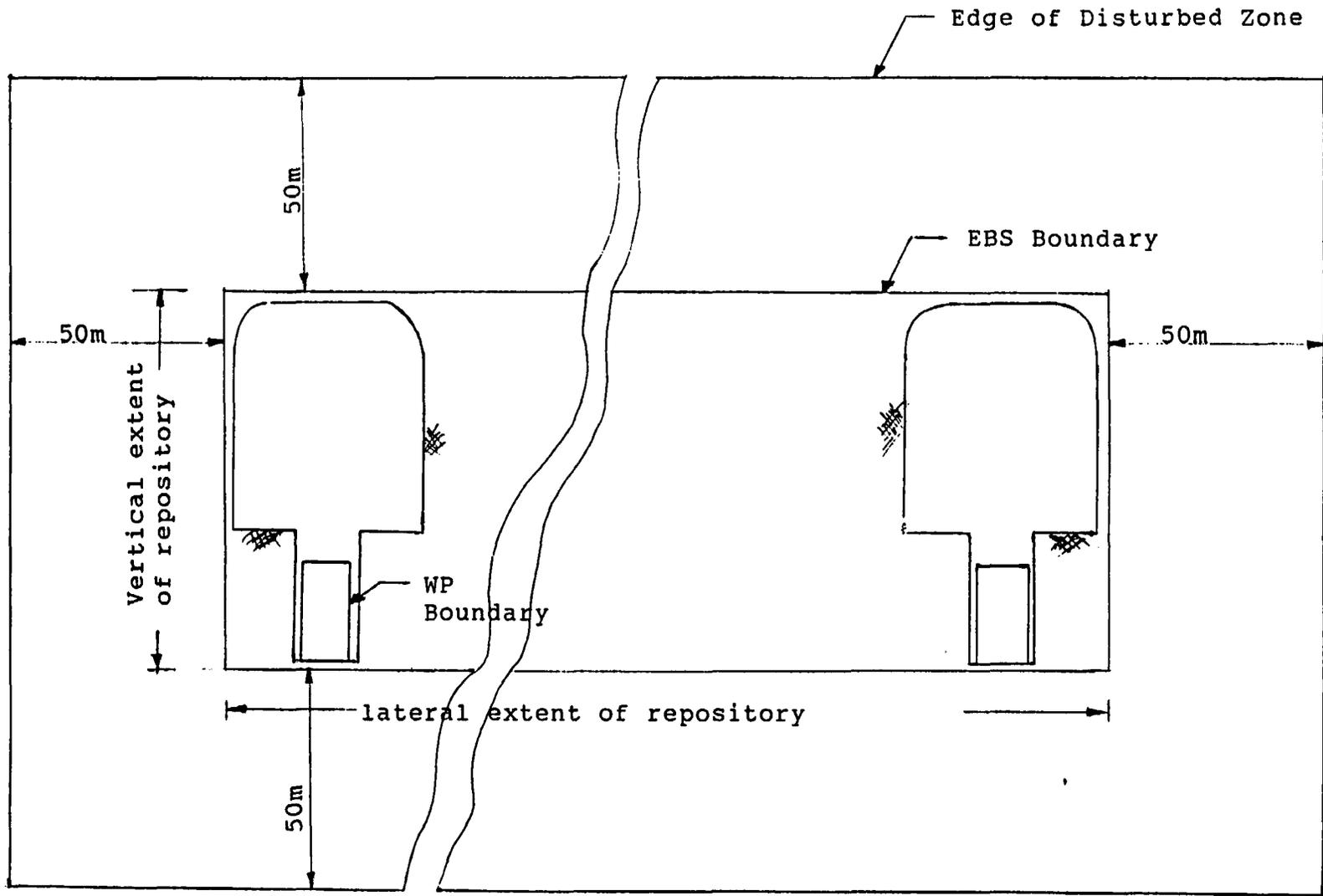


Figure 2.6 Boundaries of Waste Package, Engineered Barrier System, and Disturbed Zone.

disturbed zone. If the DOE decides to demonstrate compliance with the release rate criterion at the waste package boundary, much of the discussion that follows becomes redundant. Regardless of the choice of location at which the release rate criterion is demonstrated to comply, the processes, parameters, and properties discussed in Section 2.1.1 apply to the EBS considerations. If engineered and natural barriers contained within the EBS (but outside the waste package) are expected to control the radionuclide releases, additional considerations are necessary.

#### 2.1.2.2. Processes That Affect Performance of the Engineered Barrier System

By definition, the waste packages are included in the EBS. As such the previous discussions in Section 2.1.1 are incorporated (for the EBS) by reference. Additional issues that are relevant to the EBS are discussed below.

The same general processes that can affect the waste package performance (namely, thermal, mechanical, transport, hydrological and geochemical) can also affect the EBS performance. Specific sub-processes and phenomena that can affect the performance of the EBS outside the waste packages are not necessarily the same as those inside the waste package. For example, corrosion is a relevant process only in the waste package and not outside. In general, the spatial and temporal scales of concern are very different for the waste packages and the remainder of the EBS. Likewise, if backfill is employed in the openings its consolidation becomes a phenomenon of interest.

The long term stability of the seals (i.e., the hydrological performance) emplaced within the EBS is expected to be a function of the thermal, mechanical, and geochemical environment.

#### 2.1.2.3. Relevant Phenomena and Parameters

Thermomechanical Processes. When an opening is excavated or a borehole drilled in a rock mass, the in-situ stress distribution is altered in the vicinity of the opening. Stress redistribution occurs primarily due to the fact that stress-free surfaces and a force imbalance are created by the opening, and a new state of equilibrium must be reached. This happens by a combination of rock deformation and stress redistribution, and creates a mechanically-disturbed zone. The amount of deformation (local strain) is proportional to the elastic-plastic properties of the rock mass. Depending on the rock strength and joint (or fracture) characteristics non-linear deformation as well as rock failure may occur. Damage is also caused by blasting. The extent of blast damage depends largely on the blast method (conventional, controlled, smooth-wall etc.) and the rock strength. A knowledge of the characteristics of the particular explosive(s) used in blasting is also important in estimating the blast damage. The NRC has provided guidance in a draft GTP (NRC, 1986) for estimating the extent of the disturbed zone. Elevated rock temperatures and the associated thermal stresses can be expected to affect the performance of the EBS. However, the peak temperature changes are expected to be much lower than in the waste package. The state of stress in the near field and within the EBS will undergo changes even after closure. Backfill consolidation and temperature

gradients will result in continuous deformation and stress changes for several hundred years, possibly longer. The thermal properties (conductivity, specific heat, coefficient of thermal expansion) and mechanical properties of intact rock and rock mass (elastic moduli, compressive and tensile strength, joint characteristics) must be known for the disturbed and undisturbed portions of the rock mass within the EBS boundaries. For rocks that exhibit creep, appropriate creep parameters must be known including possible temperature dependence. Concerns related to excessive deformation are probably more relevant during operational period and are primarily non-radiological safety concerns. Nevertheless, the excessive deformation prior to closure could impact the long-term isolation capability of the adjacent rock. Therefore, proper support (rock bolts, shotcrete, liners etc.) must be designed for the operational phase in order to avoid long term consequences.

Radionuclide Transport The primary process to address in assessing whether or not a given repository will comply with the NRC standard regarding the EBS (10 CFR Part 60.113(a)(1)(ii)(B)) is radionuclide transport through the various components of the EBS via the ground water. This process is complex, varying both spatially and temporally, and is affected by many other processes that occur in the engineered barrier system.

One of the functions of both the packing and the backfill in the drifts is to inhibit the flow of water to the waste container, thereby minimizing its corrosion and the subsequent leaching (or dissolution) of the waste form. It is necessary to know how much of the water from the host rock flows through

the packing to the container. The parameters that must be considered in determining this flow process include the pore characteristics, fracture characteristics, degree of saturation and permeability of the barrier materials, as well as the density and viscosity of the water. Steam generation must also be considered, especially if the "packing" to be utilized is air. Once the transport of water through the packing is known, the corrosion rates of the container and resultant leaching (or dissolution) rates of the waste form can be estimated, given other parameters such as the geochemistry and waste form. This knowledge will help define a time-dependent source term for the calculation of the transport of radionuclides through other components of the EBS. The source term at the waste package boundary is governed completely by the performance of the waste package, as discussed previously.

Once the source term for the release of radionuclides from the waste package has been established, the transport of the released radionuclides through the backfill in drifts, and through the host rock to the edge of the EBS can be modelled. This will require combining the releases of radionuclides from individual waste packages into a single source term. In doing so, possible synergistic effects of the waste packages must be accounted for. That is, analysis of waste package performance considers an isolated waste package; analysis of the EBS performance must account for the fact that each waste package will affect the performance of the waste packages near it. Such analysis should include a temperature distribution that considers each waste package as a heat source, ground-water and water vapor flow paths that are consistent with the temperature distribution and the distribution of waste packages, the geochemical effects of having many adjacent waste packages,

which may all be releasing radionuclides, and the fact that the various waste packages are not equidistant from the boundary of the EBS.

The primary mode of radionuclide transport is via the ground water; thus, it is essential to know the ground-water flow through and around the repository. Modelling this flow requires knowledge of the hydrologic properties of the barrier materials and water, discussed above; in addition, the recharge rate to the surface and resulting flux, the pressure gradients for ground-water flow, the degree of vapor formation and the effects of this vapor on the flow of liquid water, and appropriate boundaries and boundary conditions must also be known. The correlation between some of these parameters, such as permeability and degree of saturation, should also be considered, if possible. Some of these properties may be obtained by direct measurement in the field, by experimentation in the laboratory or in the field, or may have to be assumed.

Modelling the transport of radionuclides involves first determining the flow path(s) and GWTT(s) for fluid flow to the EBS boundary. The transport of radionuclides may be inhibited either by chemical reactions in the backfill and/or rock, or by being physically retarded. Alternately, radionuclide transport may be enhanced by colloid formation, which may decrease the radionuclide travel time to the edge of the EBS. In order to estimate the extent to which radionuclides are retarded by the barriers, it is essential to know the ground-water flow through the repository and surrounding area, as discussed above, the geochemistry of these barriers and of the ground water (see Geochemical Processes), and the physical properties of the barrier materials and radionuclides that control radionuclide retardation. Physical

retardation usually occurs by the process of diffusion, either into or out of adjacent flow paths under concentration gradients, into the matrix of the rock, and/or into fluid which is not part of the bulk flow of the ground water (OECD, 1984). The properties of the barriers which are important in determining the degree of physical retardation include the pore fracture characteristics, the thickness of the barriers, and the void space in the barriers. The diffusion coefficients of the radionuclide species, and which radionuclides are present and in what amounts will also determine the extent of physical retardation. It is important to account for the depletion and production of radionuclides as a result of radionuclide decay and daughter nuclide formation, especially when considering concentration-gradient driven processes and sorption. A daughter nuclide may be sorbing while its parent may not, or vice versa. So far, radionuclide transport in the vapor phase has not been discussed here; however, some of the more volatile radionuclides may be vaporized in the near-field because of the high temperatures present and may be transported to the edge of the EBS in the vapor phase. Consequently, this mode of radionuclide transport should also be accounted for. Estimating some of the properties and parameters listed above will require one of several different approaches; those which cannot be determined experimentally will have to be estimated by modelling. Finally, geometric boundaries need to be set, and initial conditions and boundary conditions concerning the concentration of radionuclides should be established.

Although the exploratory shafts, boreholes, and their seals are not specifically a part of the EBS, radionuclide transport through the portions of these structures that are within the EBS volume should be accounted for. Some of the shafts and boreholes pass through aquifers, and are sealed at

their intersection with these aquifers to prevent the free flow of water into the repository. It may be possible, however, when seals fail that rapid inflow of water will adversely affect release rates from the EBS.

Thermal Processes that Affect Transport As with the waste package, the heat generated by the waste may have an adverse effect on the performance of (release rates from) the engineered barrier system. The area of concern with respect to heat generation is the possible change in the hydrologic properties, transport properties, and geochemistry of the backfill in drifts, and the host rock that is part of the EBS, with the resultant increase in release rates from the EBS.

In order to estimate the transient thermal response due to the decay heat of the waste, the same processes and parameters that were considered in estimating the temperature response in the waste package should be considered in the EBS. In addition, the thermal conductivity, (which may be related to water content), specific heat, density, and appropriate dimensions of the backfill and host rock should also be ascertained.

The transient thermal response provides the range of temperatures over which the transport characteristics of the various components of the EBS must be known. It is desirable, albeit difficult, to estimate the temperature dependence of the transport characteristics of the transported materials, the waste package, the backfill in the drifts, and the host rock. These characteristics are discussed in the sections pertaining to radionuclide transport and geochemistry in the EBS. For some of these properties,

techniques to measure their dependence on temperature do not exist, so this dependence should be modelled. For others, such techniques do exist, and the temperature dependence of these properties may be estimated with experiments, either in the laboratory or in the field. Some of these properties may be interdependent; consequently, this interdependence should also be assessed. A further consideration is that certain properties of the host rock may have been altered by the mining process. The temperature dependence of the properties of disturbed rock can be determined only by in-situ testing. This temperature dependence should be included in the assessment of the performance of the EBS.

Another effect of the heat generated by the waste may be the alteration of ground-water flow in and around the repository, especially through the disturbed region of the EBS. To assess these effects, it is necessary to know the properties of the water and the barriers that determine flow, as given above, and how these properties change both with temperature and with the stresses and strains imposed by mining the repository.

Geochemical Processes In the design of a repository, the geologic setting is assumed to provide the major barrier to radionuclide transport to the accessible environment. The ability of not only the host rock, but also the backfill and packing to behave as barriers may depend on, to a large extent, their geochemistry. The geochemistry of the rock and the ground water may either retard the radionuclides by adsorption, precipitation, filtration, ion exchange, or isotope exchange, or it may prevent retardation by complexation or colloid formation, although colloids can also retard radionuclide

transport. These processes are complex, but have often been simplified for analysis by assigning a constant retardation factor to each radionuclide.

Adsorption and its reverse, desorption, are complex processes dependent on the ground-water composition, Eh, pH, temperature, ionic strength, the adsorbed materials (radionuclides), and the surface area of the adsorbing material (e.g., clays, silica) available for adsorption. The process of adsorption and desorption exhibits hysteresis, which should be taken into account when modelling the process. Also, sorption can be inhibited or prevented by complexation. Therefore, the above parameters, as well as the temperature dependent rates of adsorption and desorption and the thermodynamic equilibrium constraints, should be known in order to include adsorption and desorption of radionuclides in the transport calculations.

The extent of radionuclide transport in the ground water is also governed by the solubility limit of each radionuclide in the ground water. The solubility of a given radionuclide species is a function of the temperature, the ionic strength of the ground water, the concentration of other species in the ground water, the pH, and the Eh of the ground water. The possibility of supersaturation should also be addressed.

The possibility of ion exchange with naturally occurring species should also be considered, in addition to isotopic exchange with the same element or with a different element in a solid phase. Assessing these processes requires knowledge of the chemical species present (radionuclides, ions, isotopes) in the ground water, rock, backfill, packing, and waste. The rates of these exchange reactions should also be known, which requires knowing the reactions

that can occur, the order of these reactions, the rate constants, the temperature dependence of the rates, and the equilibrium concentrations.

Colloid formation is a mechanism that should be considered in estimating radionuclide transport. This process can prevent radionuclide retardation by allowing the radionuclide to travel faster than the mean ground-water velocity, or it might actually increase retardation via ultrafiltration in the porous matrix of the rock. Colloid formation will be significant in estimating radionuclide transport only if the rock is very porous and if the pores are large enough to allow colloid passage through them, or if flow is predominantly in the fractures. Colloids are formed either by physical disaggregation or weathering (e.g., clays), or by precipitation (e.g., oxides of Si, Al, Fe). Colloids in geologic systems are typically metastable, although some are stable. The reaction of a colloid with a radionuclide may result in either a colloid in which the radionuclide is a structural component, or in a colloid onto which a radionuclide is adsorbed and could be desorbed. To estimate the effects of colloid formation on radionuclide transport, it is necessary to know the chemical composition of the packing, backfill, and host rock, and whether any of these materials have significant amounts of naturally occurring colloids. It is also necessary to know the concentration of colloids, if and how the radionuclides will react with the colloids, and the kinetic parameters, as given for ion-exchange and isotope-exchange reactions. Because modelling colloid formation is very complex (and, thus, very expensive), and because its effects may not be significant, it is often not considered in a performance assessment.

### 2.1.3. Ground-Water Travel Time (GWTT) (10 CFR Part 60.113(a)(2))

The ground-water travel time (GWTT) rule, 10 CFR Part 60.113(a)(2), is the part of the NRC's multiple barrier approach that is meant to insure the adequacy of the geologic setting for high-level radioactive waste disposal. The rule states:

*The geologic repository shall be located so that pre-waste-emplacment groundwater travel time along the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment shall be at least 1,000 years or such other travel time as may be approved or specified by the Commission.*

#### 2.1.3.1. Definition/Description

Interpretation of this rule requires the definition of several terms. The NRC has defined the following terms in 10 CFR Part 60.2:

disturbed zone - that portion of the controlled area the physical or chemical properties of which have changed as a result of underground facility construction or as a result of heat generated by the emplaced radioactive wastes such that the resultant change of properties may have a significant effect on the performance of the geologic repository

Calculation of the GWTT starting at the edge of the disturbed zone prevents undue credit from being taken for a region that may not have the same properties after repository construction or the waste is in place. Also,

complex coupled processes that could occur after waste emplacement do not have to be considered. However, determining the exact location of the disturbed zone has proved to be difficult. Currently, the NRC (1986) defines the extent of the disturbed zone as 50m from the edge of the underground facility. The EPA has defined the following terms in 40 CFR Part 191.12:

accessible environment - (1) the atmosphere, (2) land surface, (3) surface water, (4) oceans, and (5) all of the lithosphere that is beyond the controlled area.

controlled area - (1) a surface location, to be identified by passive institutional controls, that encompasses no more than 100 square kilometers and extends horizontally no more than five kilometers in any direction from the outer boundary of the underground facility, and (2) the subsurface underlying such a surface location.

Current repository designs call for the underground facility to be approximately two kilometers by four kilometers. If the controlled area was then taken to be a fixed distance from the edge of the underground facility in all directions, the distance to the accessible environment from the disturbed zone would be between three and four kilometers. However, the controlled area could be designed such that the distance to the accessible environment would be five kilometers on one side, for example in the direction of ground-water flow. Thus, the distance used in ground-water travel time calculations will most likely be five kilometers.

Additional definitions are required to interpret the ground-water travel time

rule. These include pre-emplacment waste-emplacment conditions and fastest path of likely radionuclide travel. The NRC has provided explanations of these terms in their regulatory guide on ground-water travel time (NRC, 1988a).

The term "pre-waste emplacment" is meant to refer to conditions not only prior to waste emplacment but also prior to site characterization and repository construction activities which could disturb hydrologic conditions. In addition, the NRC explicitly states that "undue credit should not be taken for relatively short-term processes". These processes include cycles of wet and dry years, local flooding, and changes in ground-water and surface-water use. In effect, the pre-waste emplacment conditions represent the long-term steady-state behavior of the system.

The term "fastest path" is defined by NRC (1988a) to be a "macroscopic" feature such as hydrostratigraphic units, zones within hydrostratigraphic units, fractures, brecciated zones, or faults. The term "likely radionuclide travel" in the rule seems to imply the need to account for transport phenomena in showing compliance. NRC (1988a) states, however, that the estimate of GWTT should be based on seepage velocities, either measured or calculated and that his interpretation does not entail many of the complexities and uncertainties associated with solute transport modelling. Thus, the combination of these statements with the wording "fastest" in the rule implies that credit for such phenomena as matrix diffusion would not be allowed.

### 2.1.3.2. Processes That Need To Be Accounted For In Assessing Compliance With The Requirement

To assessment compliance with the GWT requirement only the process of ground-water flow must be accounted for. Ground-water flow can be thought of in terms of the movement of water through complex geometries (pores or fractures within rocks) under various driving forces. Generally, ground-water flow can be divided into saturated and unsaturated flow. This distinction not only recognizes the difference in amount of void volume filled by water but also a difference in the driving forces. In the saturated zone, the major driving force is gravity. Gravity is also important in the unsaturated zone (especially under infiltration conditions); however, capillary forces are of much more relative importance than in the saturated zone. Other processes that may have to be considered include heat transfer (geothermal, not heat generated from the radioactive waste) and salt dissolution in cases where they may affect ground-water flow.

### 2.1.3.3. Relevant Phenomena and Parameters

NRC (1988a) stresses that the calculation of ground-water travel times must be based on a defensible conceptual model(s). This means that all assumptions and simplifications used to develop and implement the model must be justified. Once the conceptual model(s) has been formulated, the calculation of GWT's is a two part problem (NRC, 1988a). First the fastest path of likely radionuclide travel must be identified. This requires a combination of geologic and hydrologic data to: 1) identify hydrostratigraphic units; 2) identify zones within (or across) these units

which are the most conductive; 3) determine recharge and discharge conditions and; 4) define boundary conditions. Once the path(s) has been identified then the travel time must be calculated. This requires a knowledge of the hydraulic conductivity, the effective porosity and the hydraulic gradient along the path. This includes the spatial correlation of these parameters and the correlation between these parameters. For unsaturated conditions, the hydraulic conductivity as well as the effective porosity must be known as a function of moisture content and/or pressure. In fractured media, knowledge about the fracture apertures, spacing, orientation, and connectivity may be required to determine appropriate values of the hydraulic conductivity and effective porosity. In cases where the temperature and/or the water chemistry changes along the flow path, then the density and viscosity of the water must also be known to accurately determine the hydraulic conductivity and gradient. If the pre-waste emplacement conditions are transient, then the compressibility of both the water and the geologic medium must be known to accurately predict ground-water travel times. Additional data will be required to formulate and defend the conceptual model(s). This could include but is not limited to hydrochemical, radiochemical, and isotopic data.

The above discussion assumed that the flow system behaves as a continuum and that the classical aquifer equations based on Darcy's law (or Richard's equation for unsaturated flow) apply. In some fractured media, saturated or unsaturated, this assumption may not be valid. In that case, none of the parameters mentioned above would be valid measures of the system performance and a different formulation of the problem would be required.

## 2.2. EPA (40 CFR Part 191 and 10 CFR Part 60.112)

As dictated by the Atomic Energy Act of 1954, Reorganization Plan No. 3 of 1970, and the Nuclear Waste Policy Act of 1982, EPA was responsible for the development and promulgation of environmental standards for the management and disposal of spent nuclear fuel, high-level radioactive wastes, and transuranic radioactive wastes. These standards are prescribed in *The Environmental Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level, and Transuranic Radioactive Wastes, 40 CFR Part 191*. The implementation of these standards is the responsibility of the NRC for the management and disposal of wastes generated from commercial nuclear-power generation activities. Such implementation is described in 10 CFR Part 60.112.

The EPA standard, as 40 CFR Part 191 is referred herein, consists of two subparts (Subparts A & B). Subpart A prescribes limits of radiation exposure of members of the public during the management and storage of the wastes. Subpart B contains the different types of requirements for the disposal of the wastes. The discussion that follows is only aimed at the requirements in Subpart B because these are the ones that deal with the post-closure phase of high-level waste disposal.

Three requirements are prescribed in Subpart B. The main one deals with the long-term containment of the waste - containment requirements (40 CFR Part 191.13). It limits the releases of radioactivity to the accessible environment during the 10,000 years following permanent closure of the disposal system. Two other requirements - the individual protection (40 CFR

Part 191.15) and the ground-water protection requirements (40 CFR Part 191.16) are also contained in Subpart B. These two requirements apply only to the first 1,000 years after disposal. In addition to promulgating these requirements, EPA also provides some guidance in Subpart B for the implementation and the EPA's intended application of the standard. Finally, EPA states that these standards, although intended for geologic disposal of these wastes, may nevertheless apply to other disposal alternatives such as sub-seabed disposal.

The processes, phenomena, and parameters that are likely to have a significant impact on assessing compliance with the three requirements in Subpart B are discussed below.

### 2.2.1. Containment Requirements (40 CFR Part 191.13)

The Containment Requirements (40 CFR Part 191.13) are promulgated by the Environmental Protection Agency (EPA) and implemented by the NRC (10 CFR Part 60.112) as the performance objective for determining the suitability of an overall HLW disposal system (engineered barrier and geologic setting) to effectively prevent significant amounts of radioactivity from reaching the public. This performance objective limits the total releases of particular radionuclides caused by all potentially credible events and processes that may affect the performance of the disposal system for 10,000 years following the permanent closure of the repository. Assessment and demonstration of compliance with the containment requirements means that both anticipated and unanticipated events, as defined by the NRC (1988b), need to be considered.

The intent of the Containment Requirement is to establish release limits for radionuclides that assure that the disposal system will provide sufficiently long isolation of the wastes such that the risk to future generations will be minimal. Specifically, such risk should not be greater than the risk that would have existed if the uranium ore from which the wastes were generated had never been mined. Furthermore, this criterion emphasizes the performance of the overall system with all its components rather than the performance of individual components.

The Containment Requirements also automatically allow the estimation of risk. The cumulative probability of small releases is allowed to be higher than that of high releases. The complementary cumulative distribution function (CCDF) that must be constructed itself is not a measure of risk; however, the

area under the CCDF represents the total risk due to radionuclide releases from all credible events and processes.

In the development of the Containment Requirements, EPA assumed that the current state of the art allows the prediction of future events reasonably well so that the behavior of the disposal system can be determined based on such predictions. The 10,000-year regulatory period was chosen because EPA believed that it is sufficiently long to establish if a given disposal system is suitable or not. Conversely, EPA also advocated that 10,000 years, in a geologic time frame, is fairly short so that significant geologic changes are not likely.

To arrive at the release limits listed in Table 1 of Appendix A in 40 CFR Part 191, EPA performed analyses of hypothetical geologic repositories that were considered to be representative of the sites being considered by the DOE. According to the calculations done, EPA concluded that, if the performance objectives promulgated by NRC in 10 CFR Part 60 for the engineered barrier system are met, the disposal of approximately 100,000 metric tons of heavy metal would cause premature deaths ranging from less than ten to slightly more than 100 during the 10,000 years after closure. These analyses allowed EPA to establish that these release limits would satisfy two main objectives of the regulation, namely: (1) it provides a level of protection that seems achievable given the existing disposal alternatives and (2) it maintain risks to future generations at acceptable low levels.

#### 2.2.1.1. Definition/Description

The Containment Requirements specify that

*Disposal systems for spent nuclear fuel or high-level or transuranic radioactive wastes shall be designed to provide reasonable expectation, based upon performance assessments, that cumulative releases of radionuclides to the accessible environment for 10,000 years after disposal from all significant processes and events that may affect the disposal system shall:*

*(1) Have a likelihood of less than one chance in 10 of exceeding the quantities calculated according to Table 1 (Appendix A); and*

*(2) Have a likelihood of less than one chance in 1,000 of exceeding ten times the quantities calculated according to Table 1 (Appendix A).*

"Performance assessments" refers to the analysis that (1) identifies all potentially relevant processes and events that could affect the behavior of the disposal system; (2) estimates the consequence of these processes and events with respect to release of radionuclides; and (3) estimates the cumulative releases of radionuclides taking into account all associated uncertainties. Furthermore, EPA prescribes that the estimates of radionuclide releases shall be incorporated into a probability distribution of cumulative releases. This distribution function, the CCDF, represents the probability of exceeding multiples of the total release of all radionuclides normalized

according to the values given in Table 1 (Appendix A of 40 CFR Part 191)

Description of Performance Objective. The release limits listed in Table 1 (Appendix A of 40 CFR Part 191) represent limits for a given radionuclide assuming that no other radionuclide is released. In order to estimate the total release of several radionuclides, the requirement becomes

$$\sum_{i=1}^n Q_i/RL_i \leq 1$$

where  $Q_i$  is the estimated total release for the  $i^{\text{th}}$  radionuclide over 10,000 years,  $RL_i$  is the corresponding release limit in Table 1 (Appendix A of 40 CFR Part 191), and  $n$  is the number of radionuclides. The summation in this last equation denotes the "Normalized EPA Sum." It should be noted that the release limits in Table 1 correspond to an initial inventory generated from 1,000 MTHMs. It is necessary to adjust the release limits in Table 1 (Appendix A of 40 CFR Part 191) when the MTHMs are not exactly equal to 1,000. For example, if instead of 1,000 MTHMs, the inventory was generated from 50,000 MTHMs, then the release limits need to be multiplied by 50. Conversely, if the inventory came from 500 MTHMs, then the release limits are divided by 2.

The Containment Requirements require that in generating the CCDF, all potentially important events and processes that could affect the performance of the disposal system be considered. Typically, these events and processes are combined to form "scenarios" (see Section 3.2). The construction of the

CCDF requires that the releases resulting from each scenario be included. For example, for  $m$  scenarios, the probability of exceeding a given normalized EPA sum,  $R$ , is given by

$$P(\text{Re}|>R) = \sum_i^m P(\text{Re}|>R|S_i) P(S_i)$$

where  $P(\text{Re}|>R)$  is the probability that the release will be greater than  $R$ ;  $P(\text{Re}|>R|S_i)$  is the probability that the release will be greater than  $R$  for the  $i^{\text{th}}$  scenario ( $S_i$ ); and  $P(S_i)$  is the probability that the  $i^{\text{th}}$  scenario will occur during the 10,000-yr regulatory period.

#### 2.2.1.2. Processes that Affect Overall System Performance

In this section processes that should be considered in order to assess compliance with the Containment Requirements are discussed. The discussion also includes identification of relevant parameters associated with the processes.

**Natural Processes.** Natural processes that could effect the containment of the waste include both those that are occurring at the site at the present time coupled with those that will be caused by the waste and those that could happen in the future.

Over the next 10,000 years, some degree of climatic change will occur at any

candidate site location. The maximum amount of change probably would occur in association with a glacial cycle. Even without renewed glaciation, most areas will experience some period of wetter conditions. Wetter conditions generally will result in increased infiltration, especially if accompanied by denser vegetation that inhibits runoff or if more of the precipitation falls as snow. An increase in infiltration may increase an existing downward hydraulic head gradient, decrease an upward gradient, or raise the elevation of the water table. In areas with a strong orographic effect on precipitation, the horizontal hydraulic gradient could be increased as the elevation of the water table under the higher elevation increases more rapidly than under the lower elevations. For a repository in the unsaturated zone, an increase in the infiltration could provide additional water for canister corrosion or radionuclide dissolution and transport. In addition, the elevation of the water table could increase, thereby decreasing ground-water travel time from the repository to the water table. A rise in the water table could alter the point of discharge and decrease the distance from the repository to the accessible environment.

The licensing-assessment methodology should be capable of evaluating the effects of increased infiltration associated with an increase in precipitation on the ground-water flow system on an area-wide basis. For the unsaturated zone, the methodology should integrate two-phase flow (in both matrix and fractures), heat dissipation, radionuclide transport by all possible mechanisms, and changes in water-table elevation.

Glaciation as a process needs to be considered where a possible future continental-scale glacier could approach or override a candidate site. The

weight of the glacier could alter the in-situ stresses as the glacier approaches, when the glacier overrides, and while the glacier retreats from the site. This alteration of the stress field could conceivably open existing fractures, cause fracturing, or reactivate existing faults. Any of these results could alter the ground-water flow system.

The process of glaciation needs to be considered only for those candidate sites in previously glaciated areas and those areas likely to be glaciated by a future advance. For the appropriate sites, the methodology must be capable of determining the changes to the flow field by increases in fracture hydraulic conductivity and alteration of the flow pattern by the offset on reactivated faults.

Large-scale variations in sea level can be caused by crustal movement, changes in the amount of water in the oceans, or combination of both processes. Crustal movement can be the result of epeirogenic uplift or subsidence and the advance or retreat of continental glaciers. Changes in the amount of water in the oceans can be caused by the removal of water during the advance of continental glaciers or the addition of water during the retreat of continental glaciers.

A rise in sea level could inundate a site and/or the areas overlying the aquifers associated with ground-water flow at a site, thereby increasing the hydrostatic pressures of the flow system. The lowering of sea level could decrease the hydrostatic pressures on the flow system. If appropriate for the site, the methodology should contain techniques to determine how these changes in hydrostatic pressure would change the ground-water flow.

Hurricanes, seiches, tsunamis, and/or storms provide a short-term mechanism by which water could be introduced to a site, thereby increasing the infiltration and possibly increasing the amount of erosion. Erosion will be considered under a separate heading. Seiches and tsunamis only need to be considered for sites in coastal areas. Added infiltration could have an effect on the ground-water flow system. For a repository in the unsaturated zone, even occasional short-term increases in infiltration could be an important source of water for canister corrosion and for radionuclide transport. Because of the short-term nature of these phenomena, additional infiltration probably would not have a significant effect on the level of the water table.

The licensing-assessment methodology should be capable of evaluating the effect that increased infiltration, both short-term and long-term, will have on ground-water flow. For a candidate site at which a repository would be in the unsaturated zone, the methodology must be able to determine the effect of increased infiltration on canister corrosion and radionuclide transport.

The current rates of erosion at any of the candidate sites would not disrupt the subsurface facilities directly because of the proposed depths of the facilities and the relatively short time of regulatory concern (10,000 years). A climatic change that resulted in wetter conditions would produce competing phenomena. More precipitation would produce more runoff that would by itself cause more erosion. Wetter conditions also would produce more vegetation that would retard runoff and also stabilize the soil. The aspects of erosion that are of concern are the exposure of shafts and bore holes with

degraded or poorly emplaced seals, thereby establishing pathways for additional infiltration, and the exposure of more permeable rock or soil at the surface, thereby allowing additional infiltration. The possibility of erosion resulting in an increase in infiltration is especially important for a repository in the unsaturated zone.

The licensing-assessment methodology should be able to address increased infiltration at one or more locations at and near the repository site and to determine the effects that this increase will have on the system. Most of these locations probably will be point sources of infiltration.

Sediments at a site can be deposited by water, wind, and glacial processes. In most instances, the addition of sediments will have either no or a slightly beneficial effect on the ability of a site to contain radioactive waste. If the deposition were to result in sufficient differential loading across a site, movement on an existing fault conceivably could occur. In addition, the aperture of preexisting fractures could change. The fault zone could provide either a barrier or a conduit to ground-water flow or to infiltration. An increase in the aperture of fractures would increase the hydraulic conductivity of the unit(s) involved.

Techniques for determining the effects on the flow system of changes in hydraulic conductivity of units along localized zones need to be included in a performance-assessment methodology for sites where substantial deposition may occur.

Conditions could exist at a candidate site where mudslides, avalanches, or

landslides would block one or more drainage channels. Such blockage could result in the impoundment of a stream, river, or runoff. For a perennial stream or river, impoundment of water is likely to be of relatively short duration, because once the impounded water starts to flow over the dam, the dam will be eroded. A dam across an ephemeral stream probably will last longer than one across a perennial stream, because less water is involved and the dam is less likely to be breached. The presence of impounded water is likely to increase the amount of infiltration, especially if the impounded water covers a shaft or bore hole with failed or poorly emplaced seals. An additional source of infiltration, such as impounded water, would be especially important for a site with the repository in the unsaturated zone. This source could be a major supply of water for canister corrosion and radionuclide transport.

The licensing-assessment methodology should include techniques to determine the effect on the ground-water flow system of increased infiltration along a line or at a point. For a repository in the unsaturated zone, techniques must be included to determine the effect of increased infiltration on canister corrosion and radionuclide transport.

Because of the erosion and deposition that occurs along streams and rivers, their channels can change location under the appropriate physiographic conditions. These changes tend to be more likely to occur for perennial streams and rivers in areas of low topographic relief. Both perennial and ephemeral streams and rivers in areas with moderate to high topographic relief and areas with high rates of regional uplift tend to be deeply incised. As a result, these water courses are less likely to change the

location of their channels, although stream piracy can occur. A stream or river in a humid area generally receives water from subsurface drainage. In arid and semiarid areas, streams and rivers generally contribute to the recharge. In either instance, the hydrostatic pressure on the ground-water system under the stream or river is affected, thereby altering or potentially altering ground-water flow.

For the appropriate sites, the licensing-assessment methodology should be capable of determining the effects that changes in the locations of channels of streams and rivers would have on the ground-water flow system. In addition, the methodology should be capable of determining the effects of additional recharge on the ground-water flow in the unsaturated zone, on canister corrosion, and on radionuclide transport.

In areas where the stratigraphic sequence contains either salt or limestone, dissolution of these materials can occur. Dissolution of a sufficient amount of either material could result in subsidence of the overlying unit or units. The subsidence can affect only the overlying unit or extend to any level including to the surface. A disruption of any of the overlying units could affect the ground-water flow by providing a connection of aquifers across aquitards. Once the low permeability units that had protected the salt or limestone from dissolution are disrupted, additional dissolution may occur. If the subsidence reaches the surface, a depression would form where runoff could accumulate. The resulting ponding of water could be a source of recharge.

For the candidate sites in the appropriate geologic settings, the

licensing-assessment methodology should be capable of determining how collapse features resulting from dissolution affect ground-water flow. In addition, the methodology must contain techniques to determine the effect that additional recharge associated with collapse features that reach the surface and cause ponding of runoff will have on the flow system. For repositories in bedded salt, salt creep as a function of pressure and temperature (including heat generated by the radioactive waste) must be included as a response to the dissolution.

Both uplift and subsidence, as used here, are epeirogenic in scale, and as a result, the repository and surrounding area should remain relatively intact. Depending on the rate of uplift or subsidence and where the boundaries of the region being uplifted or depressed are relative to the location of the candidate site, the regional-scale recharge for the aquifers at and near the site could be affected.

The licensing-assessment methodology should contain techniques that permit the determination of how changes in the regional boundary conditions affect ground-water flow on a regional, local, and near-field scale.

Faulting, as used here, refers to renewed movement on an existing fault and the movement associated with the formation of a new fault. Because the formation of a new fault is a rare phenomenon, especially where faults have the appropriate orientation to relieve the imposed stresses, faulting at or near a candidate site should be assumed to occur along preexisting faults. The primary effect of faulting outside of the repository area will be on the ground-water flow system. Movement that produces a zone of high hydraulic

conductivity may have a minimal effect on the system or a substantial effect by providing a conduit between aquifers. A fault zone that has a low hydraulic conductivity could act as a barrier to flow, thereby diverting flow to other discharge locations and possibly raising the water table. A rise of the water table could be a critical factor for a repository in the unsaturated zone. Faulting that occurs through a repository could have the same effects on ground-water flow as faulting outside of the repository. In addition, faulting could result in the rupture of canisters that contain radioactive waste, thereby affecting the source term. The fault zone also could provide a pathway for ground water to circulate through the repository. Factors that affect the hydrologic properties of a fault zone include the type of movement, the amount of movement, the hydrologic properties of the juxtaposed units, the composition of the units involved, and the degree of mineralization of the fault zone caused by circulating fluids.

The licensing-assessment methodology should contain techniques that can determine what effects fault zones of various hydrologic properties at various locations in the area will have on the ground-water flow system. These effects include change in the water-table elevation, the breaching of aquitards, and the diversion of flow to other discharge locations. In addition, the methodology must contain a technique(s) to determine the effect on the source term of renewed movement on one or more faults that pass through the repository.

With the exception of candidate sites within stratigraphic sequences that contain salt, the repository at any site will be at depths where the

thermomechanical properties of the rocks will not allow ductile deformation to occur. For repositories in salt, salt creep could occur in response to other processes that alter the existing conditions. Regional flexure would result in brittle deformation as fracturing prior to the formation of larger-scale faults. Some of the fractures would be the result of extensional stresses and other fractures would be the result of compressional stresses. The presence of additional fractures could alter the ground-water flow.

The licensing-assessment methodology should contain techniques that can determine the effect of changes in fracture hydraulic conductivity on ground-water flow.

Seismic activity produces ground motion that could affect the source term, ground-water flow, and the engineered barrier system. Depending on the design of the waste package, the amount of corrosion, the degree of stress failure, and the type and intensity of ground motion, additional canisters could be ruptured to an extent that the amount of radionuclides accessible for dissolution and transport would be increased. Ground motion also could rupture components of the engineered barrier system and borehole seals, thereby possibly altering the pathway for ground-water flow to and from the repository. In addition, the ground motion could alter the aperture of fractures in the rock units resulting in a change in the hydraulic conductivity.

The performance-assessment methodology must include the capability to vary the source term, determine the effect of engineered-barrier and borehole seal

failure on ground-water flow, and determine the effect of changes in fracture hydraulic conductivity on ground-water flow and radionuclide transport.

Intrusion, as used here, refers the upward movement of magma within the earth's crust. The depth of a candidate repository is too shallow for it to be intruded by a magma body without that magma body reaching the surface. If such a body reached the surface, this phenomenon would be considered in the section on volcanism. Rather than a magma body intruding into the repository, the heat from a magma body at depth would be more likely to affect the repository system.

For a site where a reasonable probability exists that a magma body is present at depth and could move to a level in the crust that would change the thermal regime, the performance-assessment methodology must be capable of determining the effects that a heat source at depth would have on ground-water flow.

Volcanic activity occurs when magma reaches the earth's surface. The compositional rock types produced can be broadly categorized as silicic and basaltic, depending on the abundance of silica present. Silicic volcanism tends to be, but is not exclusively, highly explosive, thereby producing large amounts of ash and steam. Basaltic volcanism is less explosive, with most of the material deposited as lava flows or cinder cones.

A silicic eruption that intersected a repository would result in large-scale direct release of radionuclides to the accessible environment. An eruption within the region surrounding a site would cause a major alteration of the ground-water flow system, with additional alteration resulting from caldera

collapse. The disruption would be caused by the formation of a conduit from the magma chamber to the surface, faulting and fracturing of the surrounding rock by the explosive nature of the eruption and the adjustment of the rock to an emptying magma chamber, and the flow of ground water into the caldera and some possible leakage into the magma chamber.

Basaltic volcanism can occur (1) during the waning stages of silicic volcanism, (2) when a continental plate overrides a hot spot, and (3) in a rift formed when a continental plate overrides a spreading center. The volcanic center is the result of a dike following a fault or fracture system and reaching the earth's surface. A dike that cuts through a repository could intersect canisters and carry their contents to the surface for direct discharge to the accessible environment. Direct release also could occur from a dike intersecting the contaminant plume down-gradient from the repository. A dike could disrupt the ground-water flow system by forming a barrier to flow, by forming a sub-vertical high-conductivity zone, or by the temperature of the dike creating thermal currents or flashing the ground-water to steam.

No current candidate site is likely to have problems with silicic volcanism. As a result, the licensing-assessment methodology does not need to include the capability to account for the massive disruptions that would occur to the system. Basaltic volcanism cannot at this time be eliminated from consideration for all candidate sites. The methodology must be able to determine: (1) direct release of radionuclides to the accessible environment resulting from one or more dikes intersecting the repository and/or the contaminant plume; (2) a dike acting as a barrier to ground-water flow and

diverting flow to other discharge points; (3) a dike acting as a barrier to flow and changing the elevation of the water table; (4) a dike acting as a high conductivity zone and connecting aquifers previously isolated by aquitards; and (5) the thermal effects of a dike intruded into the saturated and the unsaturated zones on ground-water flow (to include both one-phase and two-phase flow in both the matrix and fractures).

Human-Induced Processes. The technique used for the direct sampling of material at depth for resource exploration is drilling. Inadvertent drilling into a repository can result in the release of radionuclides directly to the accessible environment if a canister or the radionuclides released by canister failure are hit by the drill bit and recirculated to the surface. Direct release also can occur if drilling outside of the repository area intersects the contaminant plume. Drilling also can alter the ground-water flow if the holes are not sealed or are poorly sealed after drilling. The drill hole can provide a pathway for ground-water flow across low-conductivity units or zones. At a location that has salt in the stratigraphic sequence, ground-water flow through the drill hole can expose the salt to dissolution.

The licensing-assessment methodology should contain the capability to: (1) estimate the location of future drill holes, (2) determine the amount of radionuclides that can be brought to the surface by drilling into a canister or contaminant plume, and (3) determine the effects of small, high-conductivity zones on ground-water flow. For sites where bedded salt is present, the methodology must be capable of determining the amount of salt

dissolution that will occur as ground water flows through a drill hole and the extent to which salt creep will close the hole.

#### 2.2.1.3. Relevant Phenomena and Parameters

Source Term. Because the Containment Requirements examine the total amount of radioactivity released to the accessible environment, one of the important models must be radionuclide transport through the geosphere. This radionuclide transport model is based on the solution of the convective-dispersive transport equation. The solution of this equation requires an inlet condition (e.g., source term); that is, the amount of radioactivity released to the geosphere at the edge of the EBS. This quantity is required in one of several forms. First, if the transport equation is solved for the concentration of radioactive compounds, the inlet condition must be in the form concentration as a function of time at a given point in space. The integral of the concentration over time for the duration of the source represents the total mass of radioactive compounds available for transport. It should be noted that in this case the total mass of each radioactive compound released to the accessible environment must be converted to curies for each of the isotopes present in order to compare the releases to the limits in Table 1 (Appendix A of 40 CFR Part 191). Second, if the solution of the transport equation is tailored to directly yield total curies released to the accessible environment, the logical form of the inlet condition should be in the form of curies per unit time. The curve for the inlet condition can have several shapes. For example, the inlet condition may represent a constant mass per unit time, a pulse, or a step function. Each

particular shape is governed by the rate at which the waste can be leached from the waste form and the rate at which leached wastes dissolve in the water within the repository. The amount of radioactivity also depends largely on the inventory contained in the waste. The combination of all the processes that determine this inlet condition are collectively known as the source term. The modelling of the source term in the assessment of compliance may not need to be as complex as may be required in assessing compliance with the Release Rate from the EBS Requirement. However, it should not be taken lightly either because it has been shown that estimate of total integrated discharge to the accessible environment is very sensitive to source-term parameters.

The initial inventory of radionuclides defines several parameters needed to specify the source term. Foremost, it defines the total MTHMs that generated the inventory. It also describes all potential radioactive decay chains and fission products comprising the inventory. This is very important information for two reasons. First, the total MTHMs are required to determine the multiplicative factor for the release limits in Table 1 (Appendix A of 40 CFR Part 191). Second, the decay chains are required to keep track, as time evolves, of radioactive decay and the amount of each radionuclide both within the repository and in the geosphere. The description of the decay chains must include enough detail that would allow the identification of multiple parents and daughters. It also should include the half life of each isotope.

Leaching is likely to be the most common mechanism for removing radioactive matter from the waste form. In chemical engineering, leaching is often referred to as solid extraction because it represents the dissolution of

soluble matter from its mixture with an insoluble substrate (McCabe and Smith, 1976). After the soluble material is extracted from the insoluble one, it must dissolve in the liquid phase (which acts as a solvent) that may come in contact with the solid phase. The dissolution process is controlled by a solubility or solubility limit (see Section 2.1.1.2). The controlling parameter in leaching is the time required for the actual extraction of a certain amount of material. This time is simply called the leach time or leaching time. The main assumption made is that the material is leached at an uniform rate during the duration of the leaching period. For example, if 10 kg of material are leached in 1 hr, then 1 kg is leached every 6 minutes. Many other processes can affect the rate of leaching. For example, the chemical nature of the soluble material and the solvent; the relative time scale of leaching compared to the rate at which the solvent moves past the mixture of soluble and insoluble solids; and temperature. The chemical state of the system is important because it governs the chemical affinity of specific solutes and solvents. This is the reason why some solutes can be extracted with some solvents and not others. The relative time scales of leaching versus flow past the solid governs the mass transfer rate at the solid-liquid interface (Bird and others, 1960). The higher the flow rate, the higher the mass transfer rate, hence, the more effective the leaching process will be. That is, more material can be leached per unit time. Conversely, if the flow is slow, mass transfer tends to be slow, and consequently, leaching is not as effective. Temperature is important because many of the parameters controlling the mass transfer mechanisms are temperature dependent. The higher the temperature, the higher the state of excitation of the system will be.

Once the soluble material is leached from the waste form it must dissolve in the liquid phase. The combination of leaching from the waste form and the dissolution in the liquid phase dictates the amount of material that will be available for transport out of the repository and into the geosphere. Solubility represents the ability of the liquid phase to dissolve solid matter. Solubility is governed by a dimensionless concentration number - solubility limit - that represents the ratio of the amount of soluble material that the liquid phase can dissolve per unit mass of liquid. As the solubility limit increases, the liquid can more readily dissolve leached solids. On the other hand, if the solubility limit is low, it becomes more difficult for solids to dissolve in the liquid. To a large extent, the relative magnitude of the leach time discussed above and the solubility limit dictate whether the source term will be either leach-limited or solubility-limited. The value of the solubility limit is, in principle, a function of temperature, and chemical state. As temperature increases, it becomes easier for a solvent to dissolve given solutes. The solubility limit is also species-specific in the sense that it depends on the chemical affinity of the solvent and the solute.

The amount of water that infiltrates the repository could reduce the concentration of radionuclides dissolved from the waste form through dilution. It has been shown that this dilution process can have a significant impact on the rate at which radionuclides are released from the repository and, hence, on the total discharge to the accessible environment (Chu and Axness, 1984).

Finally, the amount of the inventory that is accessible for transport also

dictates the total amount of radioactivity that is released to the geosphere. Typically, in the demonstration of the SNLA/NRC performance assessment methodologies the entire inventory has been assumed to be available for transport. However, it can be envisioned that in some scenarios, such as human intrusion, that only a fraction of the total inventory is accessed. For example, if a borehole is drilled through the repository it may only hit a few canisters. In this case, only the inventory contained in these canisters becomes available for transport rather than the total inventory within the repository.

Ground-Water Flow. Radionuclides are transported through the geosphere from the repository to the accessible environment in the ground water. Therefore, assessment of compliance by necessity requires a model of the ground-water flow system within and around the controlled area. Processes, phenomena, and parameters that should be considered are described in Sections 2.1.3.2 and 2.1.3.3. The major difference between the types of analyses that must be performed to address the two requirements is that the GWTT requirement is only concerned with the "fastest" ground-water flow path. Here, on the other hand, the interest is in all possible paths. Also, the GWTT requirement only pertains to pre-waste emplacement conditions whereas all plausible conditions must be addressed for the containment requirement.

Radionuclide Transport. In assessing the overall system performance of a candidate repository site, fundamental consideration should be given to those processes which govern the transport of radionuclides through each of the components of the multi-barrier disposal system. These components include

the waste package, the EBS (other than the waste package), and the geologic medium surrounding the repository. The process of radionuclide transport will be a function of the properties of the radionuclides themselves, the EBS, the location of the site, which will include the site specific geohydrology and geochemistry, and those events, processes, and scenarios that affect the performance of the site. The mechanisms and parameters relevant to transport in the waste package and the engineered barrier system have already been discussed previously and can be found in Sections 2.1.1.3 and 2.1.2.3. Therefore, the discussion here will be primarily concerned with radionuclide transport through the geologic media only.

The geologic medium essentially serves as a natural barrier to radionuclide transport from the repository to the accessible environment via geochemical and physical retardation mechanisms. As discussed here, the geologic medium is the zone ranging from the boundaries of the EBS to the boundary of the accessible environment. It will therefore include the porous geologic media, which may include saturated and/or unsaturated zones and may be fractured or unfractured, as well as all the chemical species and water contained therein.

The primary mode of transport of radionuclides from the repository to the accessible environment will be via convection and/or dispersion/diffusion mechanisms through the geologic medium in the ground water. Depending on the temperature and pressure, which will be a function of both location and time, this water may be in either the vapor or liquid phase or both. At early times, near the repository, the water may be vaporized or the physical properties (e.g., density, viscosity) and chemical properties altered significantly as a result of the relatively high temperatures involved,

whereas, under the expected conditions far from the repository and at all times, the water would be expected to have quite different properties. For this and other reasons, the mechanisms governing the transport of radionuclides in ground water could also change spatially and temporally. Another consideration necessary in modelling this transport will include knowing the distribution of ground-water velocity over the domain of interest (i.e., local or regional scale), as it will vary throughout the site. In terms of the fluid velocity,  $v$ , and diffusivity,  $D$ , the relative contributions to molecular transport by convection and by diffusion may be indicated by the Peclet Number ( $Pe = vd/D$ , where  $d$  is a characteristic length). Generally, for  $Pe$  greater than 100, convection will dominate transport and for  $Pe$  less than 0.01, transport will be dominated by diffusion. If the system contains fractures, the nature of those fractures is important in that the water may travel through fractures, matrix, or both, thus requiring the understanding of how much water is transferred from the fracture to the matrix and vice versa, by what processes this transfer occurs and how this affects radionuclide transport. This information would also be especially important for the analysis of flow and recharge in both the saturated and unsaturated zones during pluvial periods, although the mechanisms may be different. Also, it must be known if and where there exist saturated or unsaturated zones and what mechanisms for transport exist in each of these zones because they could be vastly different. Ground-water flow and, consequently, radionuclide transport will therefore be strongly dependent on the physical and chemical properties of the geologic medium hosting the repository.

The fundamental parameters that govern the flow of water and mass transfer

through a fractured, porous medium include pore structure, porosity, surface chemistry, fracture characteristics and fracture/matrix interactions. Defining the pore structure of the medium requires determination of the pore-size distribution, specific surface area and specific pore volume and may include information about pore shape, tortuosity, branching and constrictivity. Fracture characteristics include orientation, density, and aperture. The fracture/matrix interactions of interest here are those that control the flow of water and transport of radionuclides between the fracture and matrix. Properties such as wettability, permeability, hydraulic conductivity, transmissivity, capillary pressure and relative and/or residual saturation level will then be functions of the aforementioned parameters, although they can be measured independently.

Other modes of transport that must be considered include radionuclide vapor phase transport in the form of volatile species and aerosols (Smith and others, 1986; Green and Evans, 1987).

In the vicinity of a HLW repository, all of these parameters and processes can exhibit extreme variations in both time and space as the result of previously mentioned naturally occurring phenomena, phenomena related to the emplacement of the waste, and human-induced phenomena. Both temporal and spatial variations can arise from changes in temperature, pressure, radionuclide release (i.e., radionuclide concentration) and geochemistry, and, perhaps more importantly, due to heterogeneities. For example, the zone in which thermal effects are considered important could possibly extend as far as and beyond the accessible environment. Depending on the thermal properties (thermal conductivity, thermal expansion, and heat capacity) and

the thermal load at the site, these effects could have a significant impact on both the chemical and mechanical properties of geologic media. Therefore, in order to accurately model radionuclide transport through the system, it will be necessary to quantify in some way, the relative impact of these changes on those parameters and mechanisms that govern the processes. This is to say, it must be understood in what way and to what magnitude these changes will occur. In addition, the existence of temperature variations implies the need for coupling heat transfer with the mass transfer processes. In summary, formulating models to simulate radionuclide transport will require that the above parameters, processes, interactions, and/or dependencies be measured experimentally, estimated with models using information obtained from experiments, or be inferred from one another. It will also require that the initial conditions and transient boundary conditions for the temperature, pressure, and radionuclide concentration be specified.

Measurement of the parameters and processes important to radionuclide transport, however, presents several problems. What is measured in the laboratory rarely simulates what will be experienced under actual conditions, primarily because of the previously mentioned spatial and temporal variations. Although laboratory experiments may yield accurate results for a given sample or group of samples, the size of the site precludes the extraction of enough samples to fully characterize it. In addition, as the result of sample-size limitations, sample disruption, time constraints, and laboratory conditions, the experiments often do not replicate in-situ conditions. In an effort to limit these errors, field or in-situ measurements are suggested, when possible, to give more realistic results.

However, even in this case, the environment will be disturbed during the measurement process. Another possible alternative is the use of natural analogs to qualitatively predict site behavior over long periods of time.

Retardation of radionuclide transport can occur by both chemical and physical mechanisms. Chemical retardation occurs primarily via interactions of the radionuclides with the chemical species contained in the ground water and surrounding rock, whereas physical retardation is usually considered to be the process of radionuclide diffusion into the rock matrix alone. Both processes may and often do occur simultaneously.

Radionuclide species may be transported from the repository to the accessible environment via ground-water flow paths or conduits that will include the pores in the rock matrix and the fractures, if present. The diffusion or migration of the radionuclide species through the porous rock matrix will be slower than it would be through a fluid alone because of pore constrictions, pore-wall barriers and a longer diffusion path length (tortuosity). This process, when considered alone, is defined here as a form of physical retardation. This inhibition can be accounted for by adjusting the value of the diffusion coefficient so that it takes into consideration those phenomena that will decrease diffusion, but while treating the nature of the process the same (i.e., bulk molecular diffusion). The diffusion coefficient will be decreased proportionally to the porosity, which accounts for pore wall barriers and a decrease in the available mean area for diffusion, and also decreased proportionally to the tortuosity, which accounts for the longer path length. This redefined diffusion parameter is usually called the effective diffusivity,  $D_e$ . The porosity used in this definition should be

the effective or accessible porosity and not the actual porosity, which includes both open and closed pores, and is often the quantity measured in the laboratory. The constrictivity may also be included in the definition of the effective diffusivity and can be combined with the tortuosity to form a single parameter, the geometric factor (Neretnieks, 1980). Modelling radionuclide diffusion from a fluid flowing through a fracture into the adjacent matrix may also require that a mass-transfer coefficient be specified for each species to describe the boundary condition at the fracture/matrix interface. The use of a mass-transfer coefficient accounts for the effect of the flow velocity on the mass flux at the fracture/matrix interface (Bird and others, 1960). The physical retardation process may also occur as the diffusion of radionuclide species into fluid not involved in the bulk flow of the ground water.

The physical retardation process can be accompanied by or replaced by what is termed here as chemical retardation which is the molecular interactions of the radionuclides with geochemical and hydrochemical species present along ground-water flow paths. This process may be further classified as sorptive or non-sorptive retardation. Sorption can consist of both chemisorption and physisorption. The latter is a physical process; however, because its nature is due to molecular interactions, it is mentioned here to distinguish it from other physical retardation processes such as matrix diffusion. The description of the geochemical and hydrochemical effects on radionuclide transport is complicated by the complexity of the processes, the site-specificity, and spatial and temporal variations of site conditions.

The retardation or effectiveness of radionuclide transport may be

characterized by determining the radionuclide-species concentration at any point at the site. This total concentration will be controlled fundamentally by processes that include: radionuclide speciation, chemical reaction, dissolution, and sorption of the species. Evaluating and modelling the effect of each of these processes on radionuclide transport will require knowing the phenomena that govern or describe each process, and the conditions under which a given phenomenon is important.

Chemical reactions may result in the formation of a variety of products or species that, depending on their properties, may either retard or enhance the transport of radionuclides. The formation of a complex (complexation) involves the bonding of a greater than expected number of molecules or ions (ligands) to a metal atom or ion due to the valence of the ions. The mobility of the radionuclide involved in the complexation may change depending on the solubility of the complex formed relative to its precursor and whether or not the complexation involves solid phase (rock surface) molecules (i.e., if chemisorption takes place). The existence of radioactive colloids can possibly enhance the transport of radionuclides by travelling at a higher average transport velocity than the mean ground-water velocity. Other reactions which may occur include hydrolysis, oxidation/reduction, and the formation of compounds such as oxides and silicates.

All of the above reactions (excluding colloid formation) may occur at the surface of the rock during the process of chemisorption. Physisorption may also occur. The sorption process is usually quantified or described by distribution coefficients, sorption ratios, or sorption isotherms. Although description via distribution coefficients is convenient, several assumptions

are made when using them, including instantaneous adsorption and desorption, linear sorption isotherms, and single-valued sorption isotherms.

The initial radionuclide concentration available for speciation and the concentration of the species formed with these radionuclides will be determined by the dissolution rates of the waste form, the solubilities and solubility limits of each species in water, the solution volume, the vapor/liquid-phase distribution coefficients and the identity and quantity of the initial geochemical and hydrochemical species and radionuclides present. The various physical and chemical conditions of the geologic environment at the site and those conditions arising from waste emplacement could in turn control or affect further reactivity or sorptivity of the resulting or available species. Radionuclide transport can be species-specific; therefore, total radionuclide releases is a function of the species present. The formation of a given species depends on the oxidation state of the system. Consequently, the redox potential, Eh, could have a significant effect on radionuclide transport. Other properties of the system to be taken into consideration include the ionic strength, the acidity (pH), the pressure, and the temperature. The relative impact of thermochemical effects on mobility depends on the thermal properties of the medium, thermal conductivity and heat capacity, and the thermal load resulting from waste emplacement. In considering solid/liquid interactions, the contact time for sorption or reaction will be controlled by flow rate effects, ground-water velocity, and the apparent diffusivity,  $D_a$  (Neretnieks, 1980), which takes into account the decrease in the effective diffusivity due to sorption. Physically, the relative colloid-to-pore size affects colloid filtration. In addition, solid phase/liquid phase interactions can include ion and isotopic

exchange between the phases. All of the above should be considered when evaluating the geochemistry of the site and its impact on radionuclide transport.

#### 2.2.1.4. Required Techniques/Procedures

The Containment Requirements explicitly prescribed that one must consider (1) all anticipated and unanticipated events and processes affecting the performance of the disposal system; and (2) all significant sources of uncertainty. Furthermore, it is also required that the impact of all events and processes as well as uncertainties be incorporated into a CCDF that represents the probability that total radionuclide releases to the accessible environment will exceed multiples of the normalized EPA sum. The combination of anticipated and unanticipated events and processes are referred herein as scenarios. The issues associated with the development, selection, and screening of scenarios, as well as the sources of uncertainty are discussed in Sections 3.2 and 3.4, respectively. The discussion here focuses only on the construction of the CCDF.

Construction of CCDF. Once the consequences of all plausible scenarios have been estimated incorporating uncertainties in models, codes, and parameters, 40 CFR Part 191.13 requires that the results of the performance-assessment analysis be presented in a CCDF showing the likelihood that given multiples of the normalized EPA sum will be exceeded. To construct this CCDF certain criteria must be met. First, the scenarios used to generate the curve must be

mutually exclusive; i.e., scenarios cannot be interdependent. Second, the sum of the probabilities of all scenarios must be less than or equal to unity. Finally, the CCDF - or most likely a family of CCDF's - must incorporate uncertainties in the estimate of the probability of occurrence of scenarios.

## 2.2.2. Individual Protection Requirements (40 CFR Part 191.15)

The individual protection requirements (IPR) were promulgated to provide limits on individual radiation exposure for the first 1000 years of undisturbed performance following closure of a repository. While similar to the groundwater protection requirements (40 CFR Part 191.16), EPA felt it was necessary to provide for individual protection and it is important to note the differences.

### 2.2.2.1. Definition/Description

The EPA requirement 40 CFR Part 191.15 states that annual exposure of an individual will be limited to 25 millirems to the whole body and 75 millirems to any organ. These restrictions apply to the first 1000 years of undisturbed performance (i.e., no human intrusion) and, perhaps more importantly, are based on the assumption that an individual ingests 2 liters of water per day from a "significant source" of groundwater from outside the controlled area. EPA defines a significant source of groundwater as (1) any aquifer currently providing the primary source of water for a community water system or (2) an aquifer that meets all of the following five conditions:

1. is saturated with water containing less than 10,000 mg/l of total dissolved solids,
2. is within 762 m (2500 ft.) of the land surface,

3. has a transmissivity of at least  $2.9E-05 \text{ m}^2/\text{s}$  (200 gallons per day per foot) provided that,
4. each of the underground formations or parts of the underground formations included within the aquifer have a hydraulic conductivity greater than  $9.4E-07 \text{ m/s}$  (2 gallons per day per square foot), and,
5. must be capable of providing a sustained yield of  $4.4E-04 \text{ m}^3/\text{s}$  (10,000 gallons per day) of water to a pumped or flowing well.

EPA defines a community water system as "a system for the provision to the public of piped water for human consumption, if such system has at least 15 service connections or regularly serves at least 25 year-round residents". For a discussion on how all the various limits were determined, the interested reader can refer to 40 CFR Part 191.

#### 2.2.2.2. Processes Needed to Predict Doses to Individuals

Prior to the arrival of contaminated ground water at a well or surface water body, the main affective processes and parameters are those that are related to ground-water flow and transport. Those issues are addressed in Sections 2.1.3.2 and 2.1.2.3. and will not be reiterated here. Therefore the next phase of processes affecting dose to an individual can be delineated into (1) environmental transport (migration of radionuclides from the surface water

through the food chain) and (2) transport-to-man (radionuclides taken through inhalation and ingestion.) Environmental transport processes could include indirect ingestion such as using contaminated water to irrigate crops or livestock. Transport-to-man processes could be direct ingestion (via drinking water), inhalation of contaminated dust particles, or adsorption through the skin. Other factors that might affect exposure are the method of irrigation used (flood versus irrigation), type of crop grown, type of animal consumed, what part of the animal was consumed (i.e., cow's milk as opposed to some specific organ), localized surface water flooding, and local soil conditions.

### 2.2.3. Ground-Water Protection Requirements (40 CFR Part 191.16)

The EPA developed the ground-water protection requirements (GWPR) to protect ground water in the immediate vicinity of a repository. The GWPR are similar to the Individual Protection Requirements (40 CFR Part 191.15) in that they apply to the first 1000 years of undisturbed performance following emplacement of the waste. However, the GWPR apply only to certain types of ground waters and the allowable release limits are different for each type.

#### 2.2.3.1. Definition/Description

In order to accurately describe the GWPR, it is necessary to define some of the terms found in 40 CFR Part 191.16.

Class I Ground Waters. EPA (1984) defines Class I ground waters as "those that are highly vulnerable to contamination because of the hydrogeological characteristics of the areas under which they occur." EPA lists "high hydraulic conductivity" and "recharge conditions" as examples of hydrogeologic conditions that could cause ground water to be susceptible to contamination. Furthermore, Class I ground waters are characterized by one of the following two conditions (EPA, 1984):

- 1) It is an irreplaceable source of drinking water. These include ground water located in areas where there is no practical alternative source of drinking water (islands, peninsulas, isolated aquifers over bedrock) or an insufficient alternative source for a substantial population; or

2) It is ecologically vital, in that the ground water contributes to maintaining either the base flow or water level for a particularly sensitive ecological system that, if polluted, would destroy a unique habitat (e.g., those associated with wetlands that are habitats for unique species of flora and fauna or endangered species).

Clearly, there are some ambiguities in the definition. For example, terms like "substantial population" and "ecologically vital" are extremely subjective and hence difficult to define without further explanation from the EPA.

Applicability of GWPR. 40 CFR Part 191.16 states clearly that the ground water protection requirements apply only to those Class I ground waters that meet the following three conditions:

- 1) They are within the controlled area or less than 5 km beyond the controlled area;
- 2) They are supplying drinking water for thousands of persons as of the date that the DOE selects the site for extensive exploration as a potential location of a disposal system; and
- 3) They are irreplaceable in that no reasonable alternative source of drinking water is available to that population.

EPA later defines Class I ground waters that meet these three criterion as

"special sources" of ground water. Again, EPA should expect some discussion on some rules because of ambiguous terms. In No. 2 (above), reference is made to supplying water to "thousands" of persons; technically this could mean greater than or equal to 2000 but it could be misinterpreted due to its subjectiveness.

Release Limits. EPA states in 40 CFR Part 191.16(a) that the release limits from a repository for the first 1000 years of undisturbed performance to a special source of ground water shall not exceed:

- 1) 5 picocuries per liter of radium-226 and radium-228;
- 2) 15 picocuries per liter of alpha-emitting radionuclides (including radium-226 and radium-228 but excluding radon); or,
- 3) the combined concentrations of radionuclides that emit either beta or gamma radiation that would produce an annual dose equivalent to the total body or any internal organ greater than 4 millirems per year if an individual consumed 2 liters per day of drinking water from such a source of ground water.

In addition, if the radionuclide concentrations in a special source are found to exceed the limits described above even before construction of the repository, releases from the system for the first 1000 years of undisturbed performance should be such that they do not increase the average annual

radionuclide concentrations in the water pumped out of the special source by the amounts specified above.

To summarize, the ground water protection requirements decree that the concentration of radionuclides released to special sources of ground water during the first 1000 years of undisturbed performance shall not exceed those amounts specified in 40 CFR Part 191.16(a).

#### 2.2.3.2. Processes That Need To Be Considered When Assessing Compliance With The Requirement

The processes affecting radionuclide concentrations in special sources of ground water can be subdivided into two groups: behavior of the hydrologic system and behavior of the radionuclide. Each of these categories can be further subdivided into numerous subgroups.

Hydrologic System. The primary process in the behavior of the hydrologic system that affects radionuclide transport is ground water flow. This process has been described in Section 2.1.3.2 which dealt with the NRC's ground-water travel time requirement. One major difference in the analysis required for GWTT and that required for GWPR arise from the hydrologic conditions that must be addressed. In the ground-water travel time requirement, the only conditions that must be addressed is pre-waste emplacement conditions. However, in addressing the GWPR requirement, all anticipated conditions that could occur after the repository closure must be considered. The other major difference between the two requirements is that

the GWTT requirement only is concerned with the "fastest" path. Addressing the GWPR requirement makes no such distinction and therefore, all potential pathways must be considered.

Radionuclides. There are a number of processes that should be examined when predicting the potential for radionuclide transport from the repository. These have been discussed in Sections 2.2.1.2 and 2.2.1.3. The major difference between the addressing the requirement discussed in those sections and addressing the GWPR is that GWPR is primarily concerned with concentration; therefore output is more likely to be sensitive to the form of the source term. The processes and parameters related to the source term (such as initial inventory, half-life, the production of daughter products, etc.) and radionuclide mobility (like leaching, adsorption, solubility) have already been discussed in Section 2.1.1.2, 2.1.2.2, and 2.2.1.3 and will not be repeated here.

#### 2.2.3.3. Relevant Phenomena and Parameters

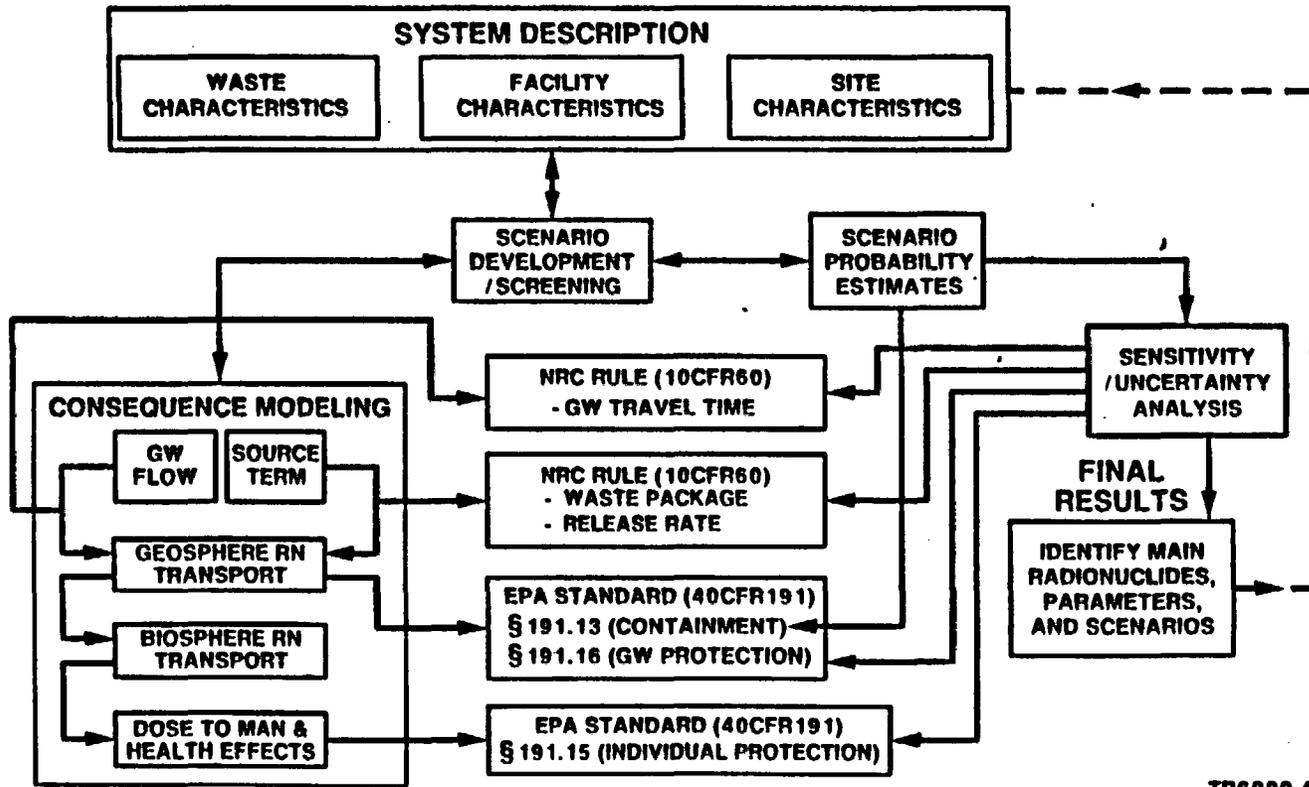
The relevant properties and parameters that relate to ground-water flow were discussed in Section 2.1.3.3. The phenomena and parameters needed to address contaminant transport are given in Section 2.2.1.3 and the phenomena and parameters that relate to the release of radionuclides from the repository are discussed in Sections 2.1.1.3 and 2.1.2.3.

### 3. OVERALL LICENSING-ASSESSMENT METHODOLOGY

In Section 2, the different processes, models, and techniques required to assess compliance with each of the six regulatory criteria for the disposal of HLW promulgated in both the EPA Standard (40 CFR Part 191) and the NRC Rule (10 CFR Part 60 ) have been discussed. In principle, it could be possible to develop a methodology to address each individual regulatory requirement; however, in reality this would be impractical. Some of the models and techniques required for a given requirement are directly applicable to others. For instance, modelling of the waste package is required for the waste-package lifetime criterion, modelling of the repository environment is required for assessing compliance with the release rate from the EBS, and a ground-water flow model is needed for estimation of the ground-water travel time, but all of these models are also needed in one way or another in the prediction of total radionuclide integrated discharges, doses and health effects, and concentrations in an aquifer.

Therefore, it is desirable to have a single overall methodology that will allow the assessment of all criteria. The basis for this methodology is the general structure of the SNLA/NRC performance-assessment methodologies. This structure, shown in Figure 3.1, is generic in nature. It is the same structure of the bedded salt methodology (Cranwell and others, 1987) and the basalt methodology (Bonano and others, 1988). It will also serve as the basis for the development of the tuff methodology under FIN A1266. It should be noticed that the consequence modelling section of the methodology is divided into several different components. These components are assembled in such a form that either they are directly used to address a specific criterion such

# METHODOLOGY FOR PERFORMANCE ASSESSMENT OF HLW REPOSITORIES



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Figure 3.1 Flow Chart for SNLA/NRC Performance Assessment Methodologies.

as waste-package lifetime or ground-water travel time, or provide necessary input for the estimation of another criterion (e.g., both the source-term and flow models feed into the geosphere transport model which is used to estimate total radionuclide discharges).

### 3.1. System Description

The first step is the description of the system which includes three aspects: namely, the characteristics of the waste, the characteristics of the site, and the characteristics of the facility. The waste characteristics include the composition and the total mass of the material to be disposed, the initial inventory (including the decay chains and fission products, and their respective half-lives), and the total metric tons of heavy metal. The characteristics of the facility consist of the size of the repository, the thermal loading, the emplacement of shafts and waste packages, and the properties of the engineered barriers. The description of the site must include the geologic structure and stratigraphy, and the hydrological and geochemical properties.

### 3.2. Scenario Development and Screening

An important component of a licensing-assessment methodology is scenario development and screening (Cranwell and others, 1987; Bonano and others, 1988). Scenarios are sets of naturally occurring and human-induced conditions that represent realistic future changes to the disposal system such that the release and transport of radionuclides are affected. Although the term "scenario" is not explicitly mentioned in either 40 CFR Part 191 or 10 CFR

Part 60 , references to the Containment Requirements (40 CFR Part 191.13) in the EPA standard and to 10 CFR Part 60.112 in the NRC rule - which requires compliance with the environmental standards for radioactivity promulgated by the EPA, i.e., 40 CFR Part 191 - are made to justify the development of scenarios.

The Containment Requirements state that an estimate must be made of the cumulative releases of "all significant processes and events" that may affect the disposal system for 10,000 years following permanent closure of the repository. By implication, all plausible combinations of events and processes need to be included also. These processes and events, either independently or in combination, represent future states of the system, and therefore, by definition are scenarios.

In 10 CFR Part 60.112, the term "anticipated processes and events and unanticipated processes and events" is used. The NRC has prepared a draft GTP (NRC, 1988b) providing guidance on the determination of anticipated processes and events and unanticipated processes and events. In this GTP, the NRC considers that the "summation of anticipated processes and events and unanticipated processes and events" is equivalent to the EPA's "all significant processes and events." Consequently, 10 CFR Part 60 requires scenarios for the overall system-performance requirement (10 CFR Part 60.112), the performance of the EBS (10 CFR Part 60.113) - although restricted to anticipated processes and events -, and in the contents of a license application (10 CFR Part 60 .21(c)(1)(ii)(C)).

Another definition in the GTP extends the need for scenarios to the EPA's

Individual Protection Requirements (40 CFR Part 191.15) and the Groundwater Protection Requirements (40 CFR Part 191.16). Both of these requirements set performance objectives for 1,000 years after repository closure based on the "undisturbed performance" of the disposal system. The EPA defines undisturbed performance as excluding only human intrusion and the occurrences of unlikely natural events in predicting the performance of the disposal system. In the GTP, the NRC assumes that "undisturbed performance" and "anticipated processes and events" have identical meaning. Consequently, the consideration of likely events by the EPA and of anticipated processes and events by the NRC requires the inclusion of scenarios to assess compliance with 40 CFR Part 191.15 and 40 CFR Part 191.16.

### 3.3. Consequence modelling

The consequence modelling portion of a licensing assessment methodology consists of (1) source term, (2) ground-water flow, (3) radionuclide transport, (4) biosphere transport, and (5) health effects. Each of these components is discussed here separately.

#### 3.3.1. Source Term

The source-term model should contain three different sub-models so that it can be used to address all the regulatory criteria involving radionuclide transport both within the repository and the geosphere. First, it could contain a detailed sub-model of a waste package to estimate its lifetime. A second sub-model in the source term could be based on the single waste-package sub-model by extending the latter to simulate radionuclide

movement within the repository and the release rate from the EBS. This second sub-model should also provide an inlet condition for the geosphere transport model needed in the assessment of compliance with the Individual Protection and Groundwater Protection Requirements. A third, less complex, sub-model should provide the inlet condition for the geosphere transport model used in estimating total radionuclide releases.

### 3.3.2. Ground-Water Flow

A ground-water flow model is required for assessing compliance with the ground-water travel time criterion in 10 CFR Part 60 . Simultaneously, the ground-water flow model will provide a description of the flow field to be used in the simulation of radionuclide transport through the geosphere needed for all three criteria in 40 CFR Part 191. The same level of sophistication should be required in the ground-water flow model for all these purposes (Bonano and others, 1988).

### 3.3.3. Geosphere Transport

The geosphere transport model is needed to estimate the rate of migration of radionuclides from the edge of the EBS through the controlled area and the total amount of radionuclides crossing the boundary of the accessible environment. Therefore, it is needed to assess compliance with the Containment Requirements. In addition, this model could also be used to estimate concentrations that will be used as input to the biosphere transport

model needed for the Groundwater Protection Requirements and/or to assess compliance with the Groundwater Protection Requirements. The main difference in using the geosphere transport model to estimate total releases versus concentrations arises through the relative importance of dispersivity. Total releases may not be too sensitive to dispersivity but concentrations are (Cranwell and others, 1987).

#### 3.3.4. Biosphere Transport

A biosphere transport model is needed to accept input concentrations from the geosphere transport model and simulate the movement of radionuclides within the accessible environment. This model will estimate concentrations in soil, surface waters, and sediments, to name a few. It may also be used to estimate uptake by humans due to ingestion, inhalation, and direct exposure.

#### 3.3.5. Dosimetry

Finally, a model to estimate doses to the entire body and to critical organs is required to assess compliance with the Individual Protection Requirements in 40 CFR Part 191.15.

### 3.4. Uncertainty Analysis

The NRC and the EPA use the terms "reasonable assurance" and "reasonable

expectation" in 10 CFR Part 60 and 40 CFR Part 191, respectively, to mean that, after considering all relevant uncertainties in the analyses, the disposal system meets the different regulatory criteria. Therefore, techniques and procedures are needed to address and reduce, to the extent practicable, the uncertainties. One aspect of addressing uncertainty should attempt to quantify uncertainties and estimate their propagation to the prediction of given performance objectives. Another aspect includes the reduction of uncertainty. A licensing-assessment methodology should by necessity include means for determining whether a license applicant has developed the necessary approaches to address uncertainty and has reduced the uncertainty to the extent practicable. This methodology also should include approaches for ascertaining whether significant uncertainties have been ignored.

At present three general sources of uncertainty have been identified (Bonano and Cranwell, 1988). These are: (1) scenario uncertainty, (2) modelling uncertainty, and (3) data and parameter uncertainty. Modelling uncertainty is further subdivided into (1) conceptual model uncertainty, (2) mathematical model uncertainty, and (3) computer code uncertainty. Of all these sources of uncertainty, data and parameter uncertainty has received the most attention to date because it can be propagated through the analysis and its effect on the estimate of a given performance measure quantified. Below all three sources of uncertainty are discussed. The discussion is an excerpt of the paper by Bonano and Cranwell (1988).

#### 3.4.1. Scenario Uncertainty

To assess the long-term performance of HLW repository, the various states that the repository may experience during the regulatory time frame needs to be postulated. Scenario development is aimed at this issue as discussed in Section 3.2. As used there, a scenario is a combination of anticipated and/or unanticipated events and processes, either natural, human, or repository induced, that could result in the release of radionuclides from the underground facility, their migration through the geosphere and biosphere, and their eventual exposure to humans. Scenario development is discussed by Cranwell and others (1988). Sources of uncertainty in scenario development include (1) uncertainty associated with the "completeness" of scenarios, (2) uncertainty associated with the estimate of the probability of occurrence of a specified scenario, and (3) uncertainty associated with the estimation of the consequences of a scenario. The latter results in uncertainty in the conceptual model for a scenario, uncertainty in the mathematical models representing relevant phenomena and associated computer codes, and uncertainty in the data and parameters required by the models and codes.

"Completeness" in scenario development refers to the uncertainty that all possible scenarios have been considered. Proof of completeness is not possible in the sense that unequivocally all possible scenarios have been considered. The only avenue to address the uncertainty associated with completeness is to develop logical procedures for scenario selection (Cranwell and Helton, 1980, 1981).

The nature of the scenarios that need to be hypothesized is such that

assigning the probability of occurrence to scenarios is quite difficult. Uncertainties associated with probabilities can be grouped into either numerical or relative depending on the approach used to arrive at the probabilities. If sufficient data are available to calculate the probabilities, the uncertainty is said to be numerical, whereas probabilities estimated based on expert judgment are said to have relative uncertainties.

### 3.4.2. Modelling Uncertainty

As mentioned earlier, modelling uncertainty encompasses uncertainty in the formulation of a conceptual model of the disposal system for a given scenario; uncertainty in the mathematical model used to represent the conceptual model; and uncertainty in the implementation of the mathematical model in a computer code. Each of these sources of uncertainty is discussed below.

#### 3.4.2.1. Conceptual Model Uncertainty

Given a scenario, the state of the disposal system must be hypothesized. This requires the formulation of a conceptual model that describes the physical and/or chemical processes taking place, the variables that relate to these processes including boundary conditions, and the spatial and temporal scales of the assumed processes. Uncertainty is introduced in performance assessment calculations when assumptions are made regarding the behavior of the system. The development of a conceptual model implies simplifying the

real system so that it can be represented with a tractable mathematical model that, in turn, can be solved using available analytical or numerical techniques. In addition, typical "real systems" are poorly described making the development of a conceptual model a formidable task. Both of these factors contribute to the uncertainty in the development of a conceptual model. If several models are developed, methods must be developed for reconciling differences among the model outputs.

#### 3.4.2.2. Mathematical Model Uncertainty

A mathematical model must be constructed after a conceptual model has been formulated. This model must describe relevant processes in order to predict the performance of the disposal system. Uncertainty in mathematical models will arise from various sources: (1) a lack of knowledge regarding the important processes and associated couplings; (2) a limited capability to mathematically represent the processes and their couplings; (3) insufficient data to describe both the processes acting on the system and the system itself; and (4) the extrapolation of the models to temporal and spatial scales beyond those for which they are tested.

#### 3.4.2.3. Computer Code Uncertainty

Sources of uncertainty associated with computer codes include coding errors, computational limitations, and user error. Computational errors can be caused by truncation errors due to finite word lengths. Another potential source of

computational errors is the use of imported numerical algorithms with data beyond the required range for a particular algorithm. The computer codes typically used in performance assessment are particularly susceptible to user error because of the complexity required to model the relevant processes in HLW disposal.

### 3.4.3. Parameter and Data Uncertainty

After the modelling problems have been addressed, one is faced with the problems of obtaining suitable values for the parameters in the models from experimental data.

Uncertainty associated with parameter values comes from several sources including (1) measurement error, (2) paucity of data, (3) misinterpretation of data, (4) spatial variation of parameters, (5) assumptions regarding the behavior of the systems, and (6) the experiment(s) is(are) not representative of the real system. Furthermore, quantifying these uncertainties in order to quantify the uncertainty in the predictions of the models can be difficult.

Measurement errors come from a variety of sources. First, the the measuring technique may be either incorrect or misapplied. Second, there is measurement error caused by the spatial variation of the data. Data often exhibit significant scatter across a site due to the spatial variability of rock properties. These properties typically vary in space even if they are measured without error. Uncertainty is introduced by replacing variable

parameters with lumped parameters or by representing a random variation with a deterministic but distributed parameter. A third source of measurement error arises because the parameters typically required by performance assessment models cannot be measured directly. Rather, their values are inferred indirectly from excitation-response data using a given equation. Uncertainty is introduced if this equation is not valid for the system of interest.

Even though different sources of data and parameter uncertainty have been mentioned here, in practice it is not possible to distinguish among them and assign a relative contribution to the total uncertainty in data and parameter to each source.

#### 3.4.4. Treatment of Uncertainty

After the sources of uncertainty have been identified, approaches for treating and/or reducing these uncertainties must be developed. Bonano and Cranwell (1988) discuss existing approaches for addressing these sources of uncertainties. In the cases where procedures do not exist, they have presented ideas about how the problem can be addressed.

##### 3.4.4.1. Treatment of Data and Parameter Uncertainty in Performance Assessment

Currently the most widely used approach for quantifying uncertainty in data

and parameters in performance-assessment analyses for HLW disposal is based on statistical analysis methods which would usually result in the construction of a cumulative distribution function (CDF) for the performance measure of interest- call it Y. The CDF is also sometimes called a distribution function (DF). Y might be the ground-water travel time (GWTT) or the total radionuclide release, for example. The CDF (or its complement, the CCDF) can give one an estimate of the probability that the GWTT, for example, is less than or equal to (greater to) a given time. The CCDF can incorporate the uncertainties of many of the parameters which influence the performance measure of interest. Thus, if methods are available or are developed for estimating the CCDF, one can make a judgment on whether specific performance objectives in the EPA Standard and/or the NRC Rule are met or not. Constructing a CCDF for a specific dependent variable, in our case a performance measure, and obtaining various statistics associated with the distribution is a part of uncertainty analysis. A methodology for generating the data required to construct a CCDF can be pictorially represented as given in Figures 3.2 - 3.4. The Y variable in the figures is summed normalized releases to accessible environment, but the figure would be the same for other Y's such as GWTT.

Uncertainty is associated with the different components in Figure 3.2. For example there is uncertainty associated with the Scenario part of the problem. The "i" in the scenario box is an index for the collection of scenarios. Each scenario will potentially have its own modelling work. The modelling work will have uncertainty associated with it as discussed above. The boxes labeled Model A, Model B, and Model C indicate the models that are generated from the modelling work for the  $i^{\text{th}}$  scenario, including computer codes.

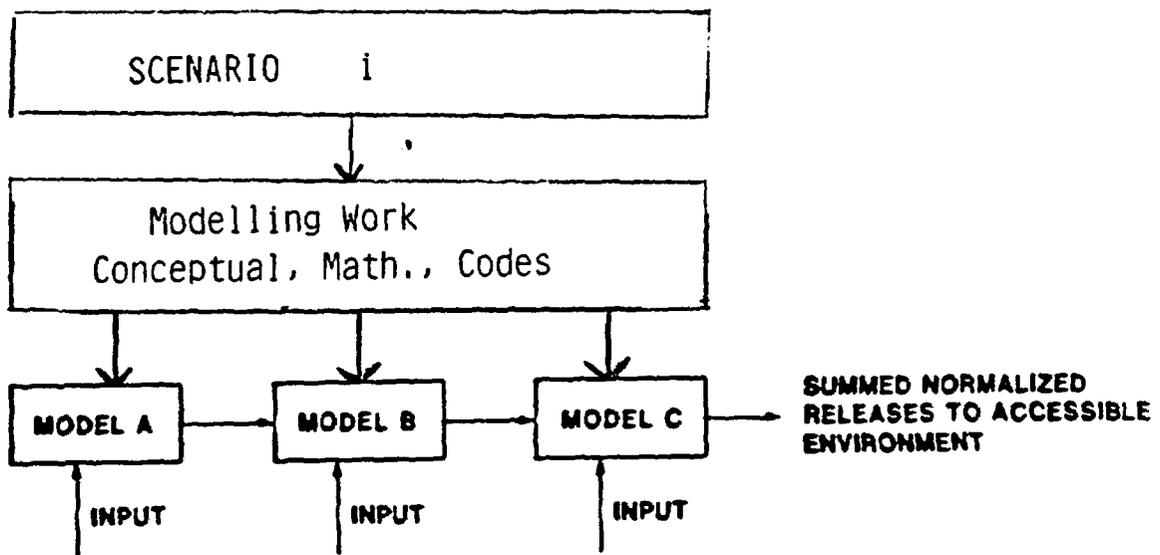
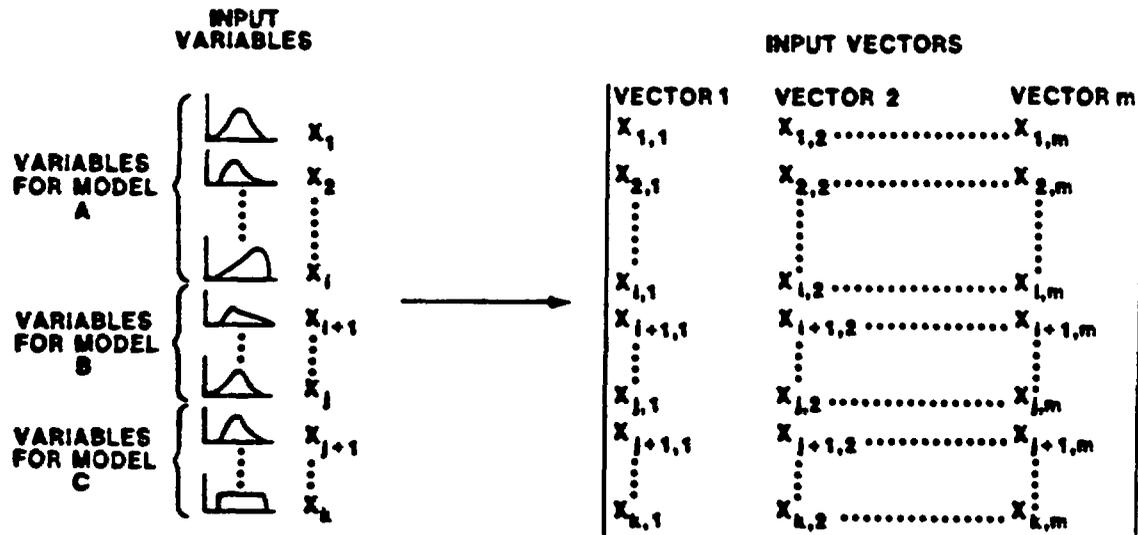


Figure 3.2. System of three models

Figure 3.3. Generation of input vectors.



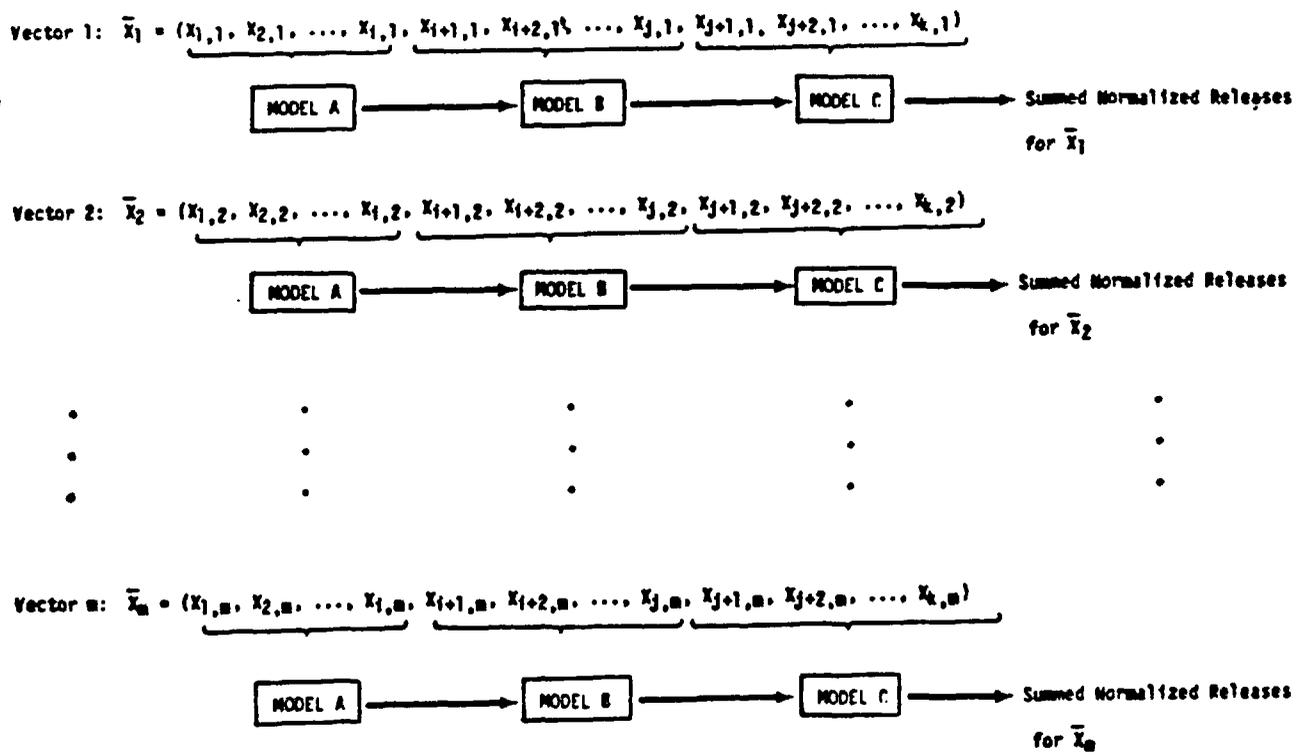


Figure 3.4a. Generation of output values for a three-model system.

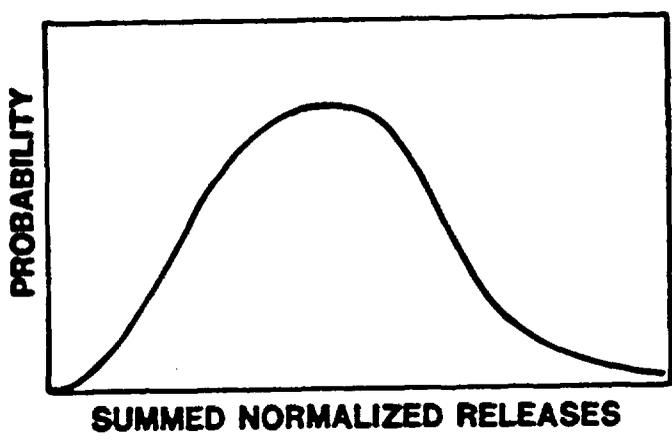


Figure 3.4b. Distribution of summed normalized releases for a given scenario.

The input variables are indicated in Figure 3.3. Distributions are shown for each input variable. The distributions can be used to capture the parameter uncertainty discussed above. How these distributions are constructed is an open question at this time. They will, no doubt, be based on data (often a very limited amount), engineering judgment, and expert opinion. Expert opinion is discussed by Bonano and Cranwell (1988). The distributions may also be interrelated. If a variable  $x_i$  is "large", another variable  $x_j$  may also have a tendency to be "large". The input variable distributions will be sampled to obtain input vectors for the models. The sampling of the input distributions will be according to some scheme - random sampling, Latin Hypercube sampling, or some other scheme. An input variable can vary spatially and/or temporally. How this type of variability affects the output variable needs to be considered. Each of the  $m$  input vectors will be used as an input to the models and a  $Y$  value will be obtained for each input vector. This aggregate of  $Y$ 's can be used to estimate the probability density function of  $Y$  and/or the CCDF.

It should be mentioned here that the regulations do not explicitly delineate methods for expressing uncertainty nor do they state - except the Containment Requirements - that a CCDF is the only way to do uncertainty analysis. Although there may be alternative methods for expressing uncertainty, a well constructed CCDF can be helpful in expressing uncertainty and judging if a performance measure meets the performance objectives.

### 3.5. Sensitivity Analysis

Uncertainty analysis can provide information on the likelihood that a given performance objective will be met; however, uncertainty analysis does not indicate which parameters contribute the most to the uncertainty in the estimate of a performance measure. Sensitivity analysis can be used to provide this latter type of information.

Neither 10 CFR Part 60 nor 40 CFR Part 191 requires that DOE perform sensitivity analyses and submit the results in a license application for a HLW repository. Nevertheless, sensitivity analyses can be very useful particularly during the site characterization process and prior to a license application. They can point out important contributors to the uncertainty in the estimate of performance measures and, hence, be used to identify areas in need of further investigation. Sensitivity analyses can also provide guidance with respect to the level of complexity required in performance assessment models. Most likely sensitivity analyses may provide the only link between research and performance assessment models and codes. If the philosophy that performance assessment and site characterization should be interdependent is accepted, then sensitivity analysis is a critical component of a licensing assessment methodology.

There are several approaches described in the literature for performing sensitivity analysis. The two main classifications are: (1) regression analysis approach and (2) deterministic approach. In performance assessment, the regression analysis typically occurs at the tail end of an uncertainty analysis using Monte Carlo simulations. Input parameters are statistically sampled leading to multiple sets of values of these parameters. For each set of input parameter values, a simulation is performed with the model(s) and

associated computer code(s) which yield a value of the performance measure(s) of interest. Thus, for each set of input parameter values, a value of the performance measure(s) exist(s). This is the case because the models conventionally used in Monte Carlo simulations are deterministic. Treating the input parameters as the independent variables and the estimated performance measure(s) as the dependent variable(s), the analyst performs a regression analysis using statistical tools in an attempt to find a relationship between them (Iman and others, 1978). The objective is to determine a set of unknown coefficients called "sensitivity coefficients". It should be noted that the expression resulting from the regression analysis does not take into account the physics relating the independent and dependent variables. If the real relationship between the independent and dependent variables is linear, or nearly linear, then the fitted expression should reproduce fairly well the true relationship. If, on the other hand, the actual relationship between the variables is highly nonlinear, then care must be exercised by the analyst in the interpretation of the results.

The second approach, the deterministic approach, takes the physics into account. In this approach, the analyst uses the actual model describing the physics to estimate the sensitivity coefficients. The latter are partial derivatives of the output of the model with respect to each of the input parameters - for this reason, this approach is also referred to as the "differential analysis" approach. The partial derivatives indicate the relative importance of each input parameter in influencing the estimate of the output. There are different approaches for estimating these partial derivatives. If the physical model is relatively simple, the partial derivatives can be determined analytically. For more complex models, the

derivatives are often estimated numerically. In recent years, the adjoint method has received much attention because it allows the determination of the derivatives in a fairly elegant manner (Harper, 1983; Cacuci, 1986). The deterministic or differential analysis approach has one main advantage over the regression analysis approach; it produces the sensitivity coefficients in a single run of the model or computer code. On the other hand, it also has some disadvantages. Among these are: (1) it is generally more difficult to implement; (2) it only estimates the sensitivity coefficients in the vicinity of a local "design point"; and (3) it is not generally suitable for multiple models and/or codes. Pin and others (1986) describe the GRESS (Gradient-Enhancement Software System) which is a FORTRAN compiler using computer calculus to automatically add the capability of estimating the partial derivatives to a computer code. GRESS considerably simplifies the implementation of the deterministic approach. Similar to GRESS, another FORTRAN compiler called ADJEN has been developed to implement the adjoint method during the compilation of a computer code (Worley and others, 1987). There are some indications that new versions of ADJEN allow the method to be applied to a series of codes in which the output of one code produces the partial derivatives that can be supplied as input to the following code (Harper, 1988) making the deterministic approach somewhat more amenable to performance assessment than it was in the past. However, it must be noted that the price that must be paid by using GRESS and/or ADJEN is substantially longer computational times. In addition, these advances have not eliminated the main drawback of the deterministic approach - the results are only valid near the design point. If the system behaves linearly, then the location of this design point should not be too critical. However, on the other hand, if the system exhibits nonlinear behavior then sensitivity analyses based on the

deterministic approach are highly dependent on the location of the design point. In this case, the analyst may need to perform Monte Carlo simulations varying the location of the design point obtain more global results.

### 3.6. Quality Assurance

Quality assurance requirements for the process of applying the license assessment methodology must be developed for assuring confidence in results obtained with existing software. Conventions, standards, and practices should be defined that are applicable to the specific activities involved. These activities include but are not limited to model and computer code selection, use and maintenance, data entry, and analysis of results.

### 3.7. Licensing Assessment Methodology Tracking System (LAMTRAX)

This section of the report deals with the development and implementation of a tracking scheme for monitoring the status of computer codes and parameters essential to the licensing assessment methodology (LAM). The licensing assessment methodology tracking system (LAMTRAX) is a user-friendly database management system designed to allow the technician to review data needs, areas needing further development, and parameter uncertainty associated with the methodology. In Section 3.7.1, the structure and design of the system are discussed. In Section 3.7.2, the actual implementation procedures are reviewed.

### 3.7.1. LAMTRAX Organizational Structure

The tracking scheme is well suited for a hierarchical organization (tree structure). Figure 3.5 is a flow chart that depicts the overall design of LAMTRAX. This figure gives only a basic overview of the structure; an example outline of the system as it currently exists is listed in Table 3.1. Basically, the system is designed around the six requirements defined by the NRC regulations (10 CFR Part 60 ) and the EPA regulations (40 CFR Part 191), with an increasing degree of complexity at each level of the structure. When the system is operational, the user will be able to easily review all of the different components of the methodology or to go directly to a given area of interest.

### 3.7.2. LAMTRAX Implementation

This section of the report proposes how the tracking system for the licensing assessment methodology will be implemented. The system design described in Section 3.7.1 is very hierarchical in its structure. This tree structure lends itself well to an interactive menu-driven environment for retrieval of information. Sandia has developed LAMTRAX and proposes to implement it on an IBM PC/AT or compatible environment using dBASE III Plus\* (Version 1.1) as

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\* Ashton Tate, 10150 West Jefferson Blvd., Culver City, CA 90203

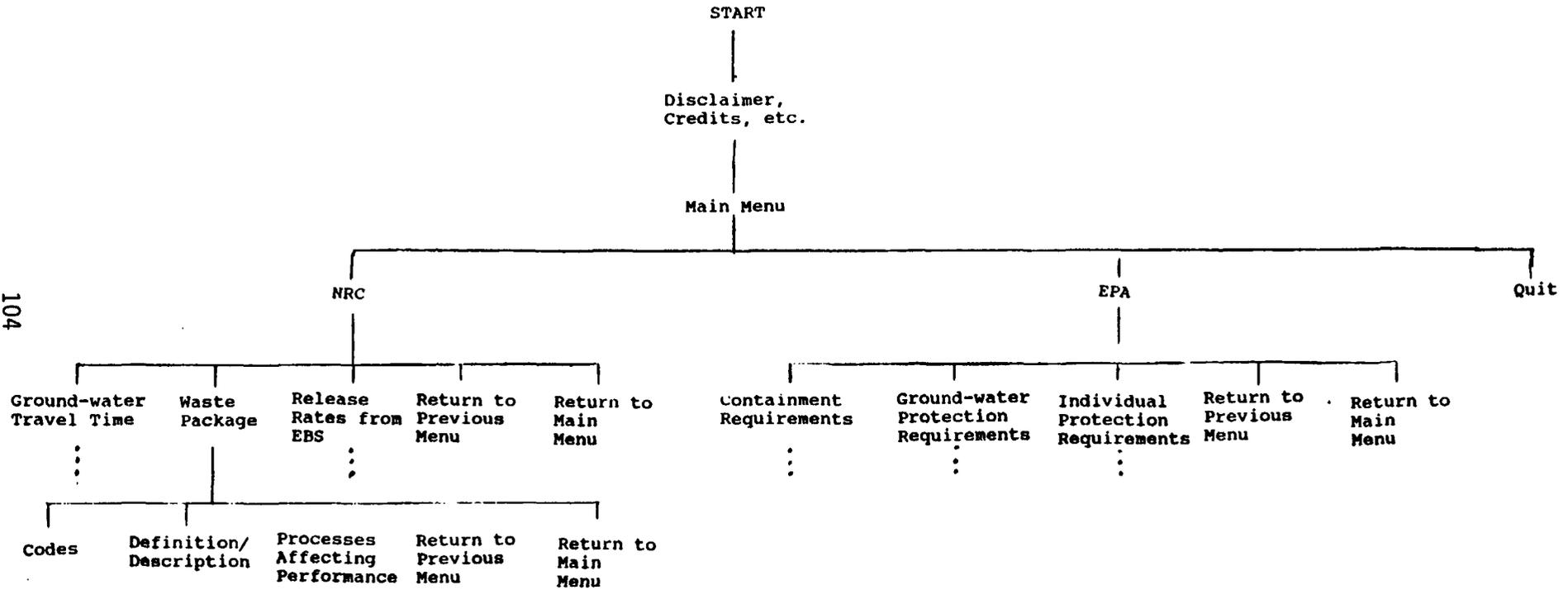


Figure 3.5 Overall Structure of LAMTRAX Design  
 (Dotted lines indicate that what follows is similar to that for Waste Package.)

the software for the database management system. This version is not copy-protected as is the case with earlier versions of dBase III. The ability to install dBASE III Plus on a hard disk with no copy protection permits start-up without first having to insert the master disk. In addition, back up of all system software is made possible.

Although dBASE III Plus is a relational (two-dimensional table) database management system, the tree-structured nature of the information can be achieved by linking multiple databases. dBASE III Plus is a proprietary software package that is acceptable to the NRC/Office of Resource Management and contains the query language and programming features of its command language that allow an interactive, user-friendly, menu-driven system to be developed. Figures 3.6-3.11 give examples of the kind of information a user might expect to see on the screen when accessing LAMTRAX. Since it is impossible to show the entire tracking system in this manner, the waste package branch (Section 2.1.1 in Table 3.1) of the structure was chosen for an example. In this case, structure given is: Main Menu -> NRC Requirements -> Waste Package -> Parameters Affecting Performance -> Waste Form -> Type of Fuel. The final system will be a detailed implementation of all six requirements. Screen forms will be developed to allow editing of the existing information contained in the system when necessary. Retrieval of components, parameters, computer codes, and other information that are part of the LAM will be achieved through the use of nested menus and will require no knowledge of the structure of the database by the end user.

Documentation of the final version of LAMTRAX will be provided in the form of

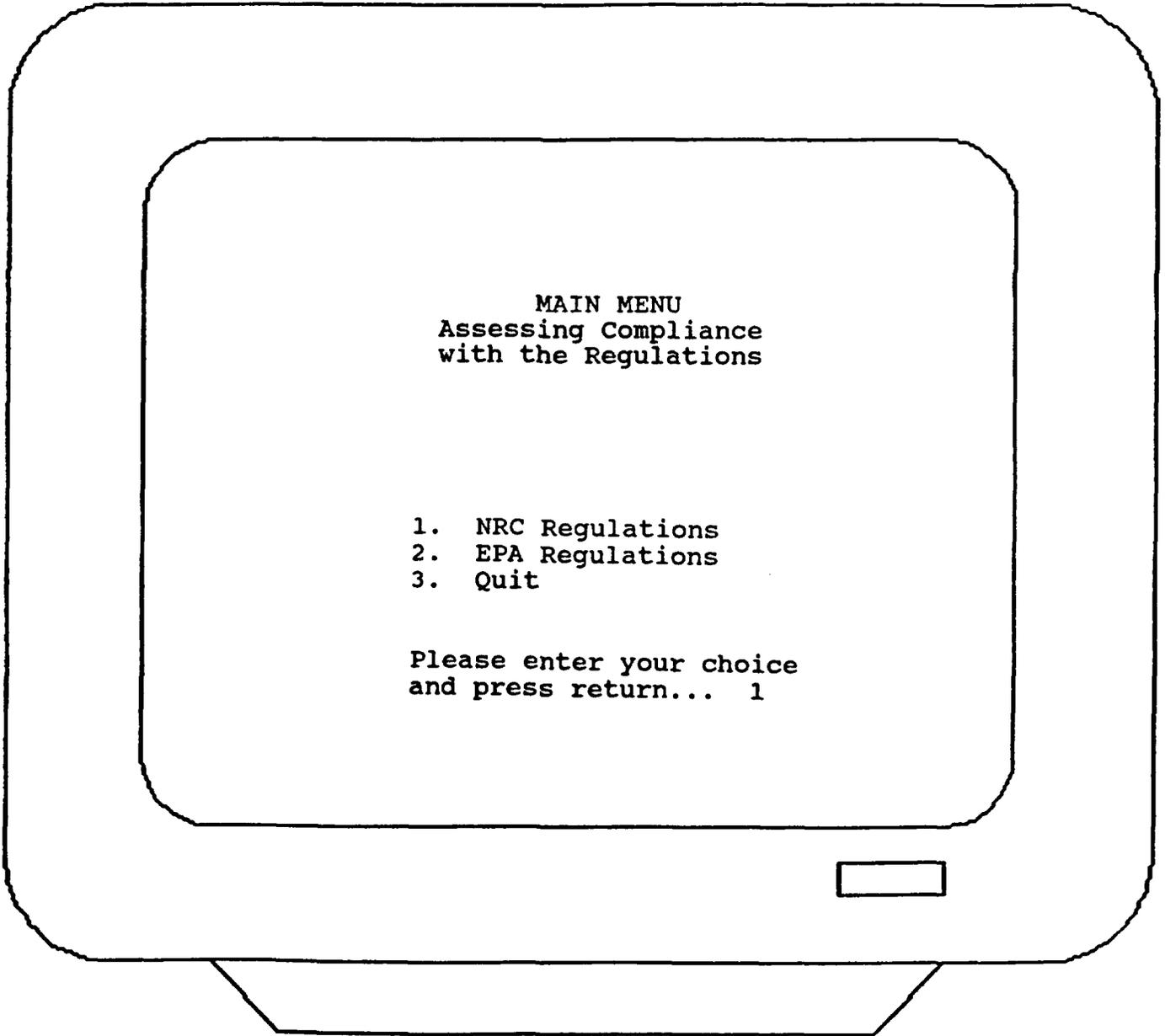


Figure 3.6. Sample LAMTRAX Main Menu

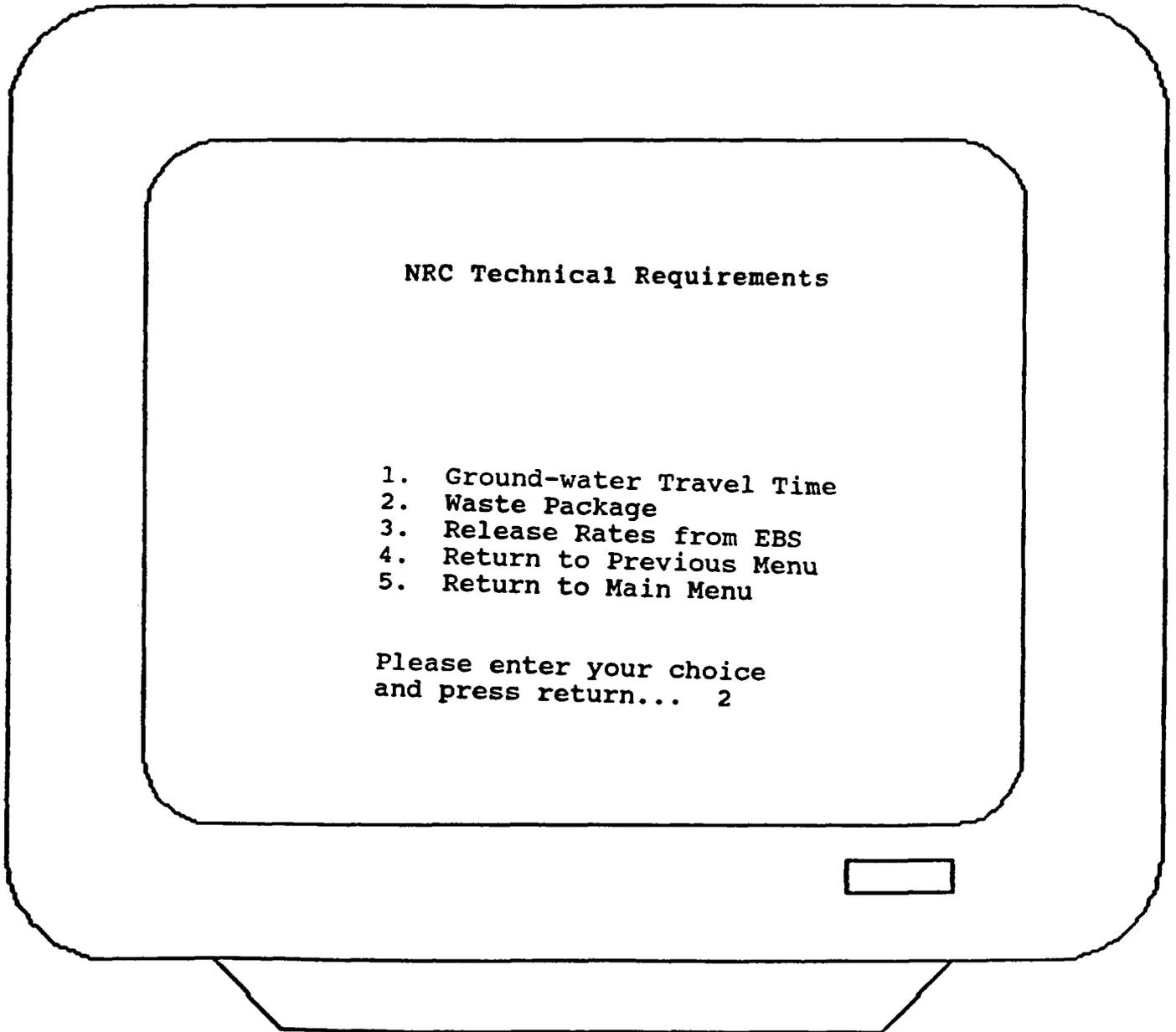


Figure 3.7. Sample LAMTRAX NRC Technical Requirements Menu

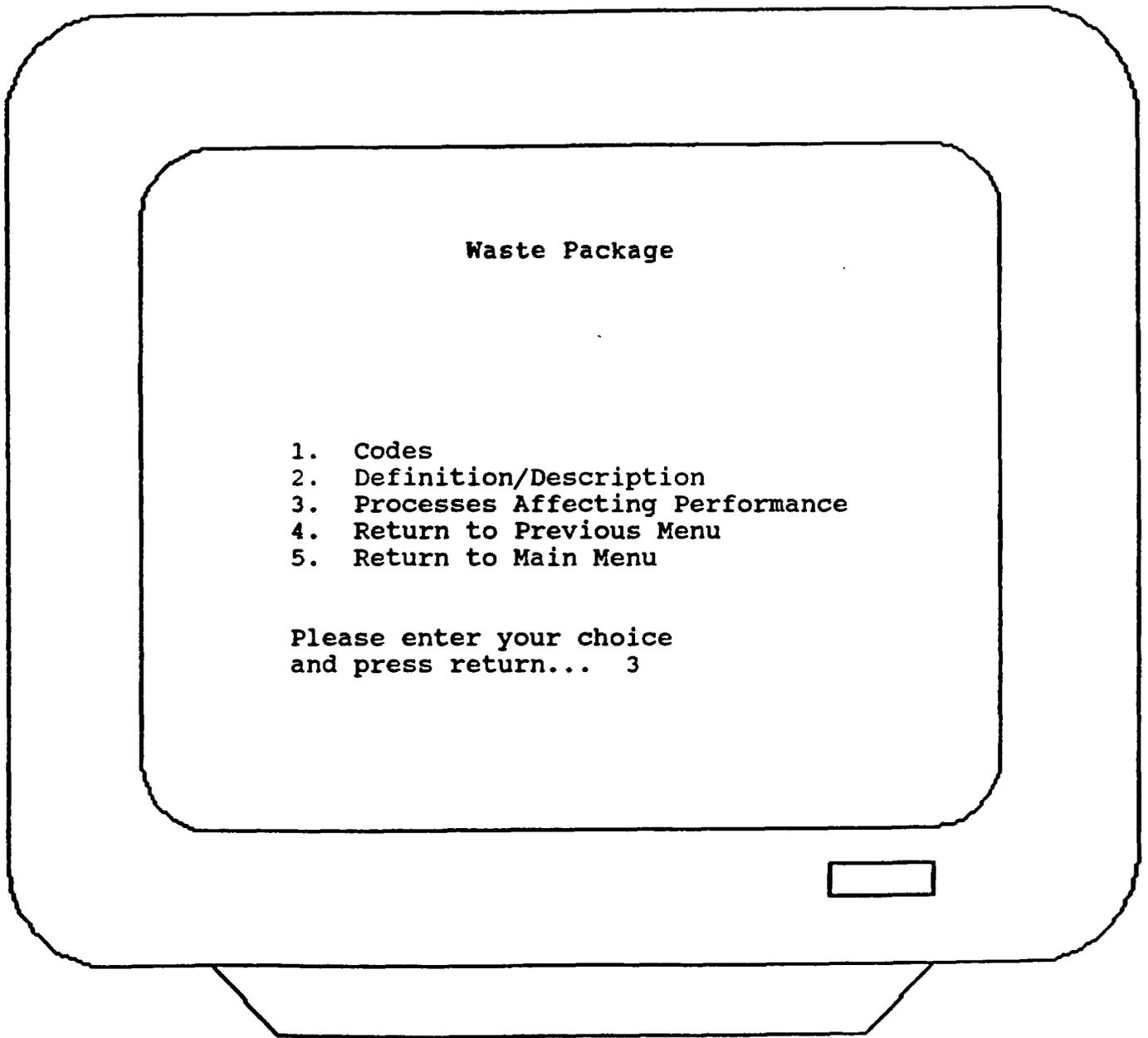


Figure 3.8. Sample LAMTRAX Waste Package Menu

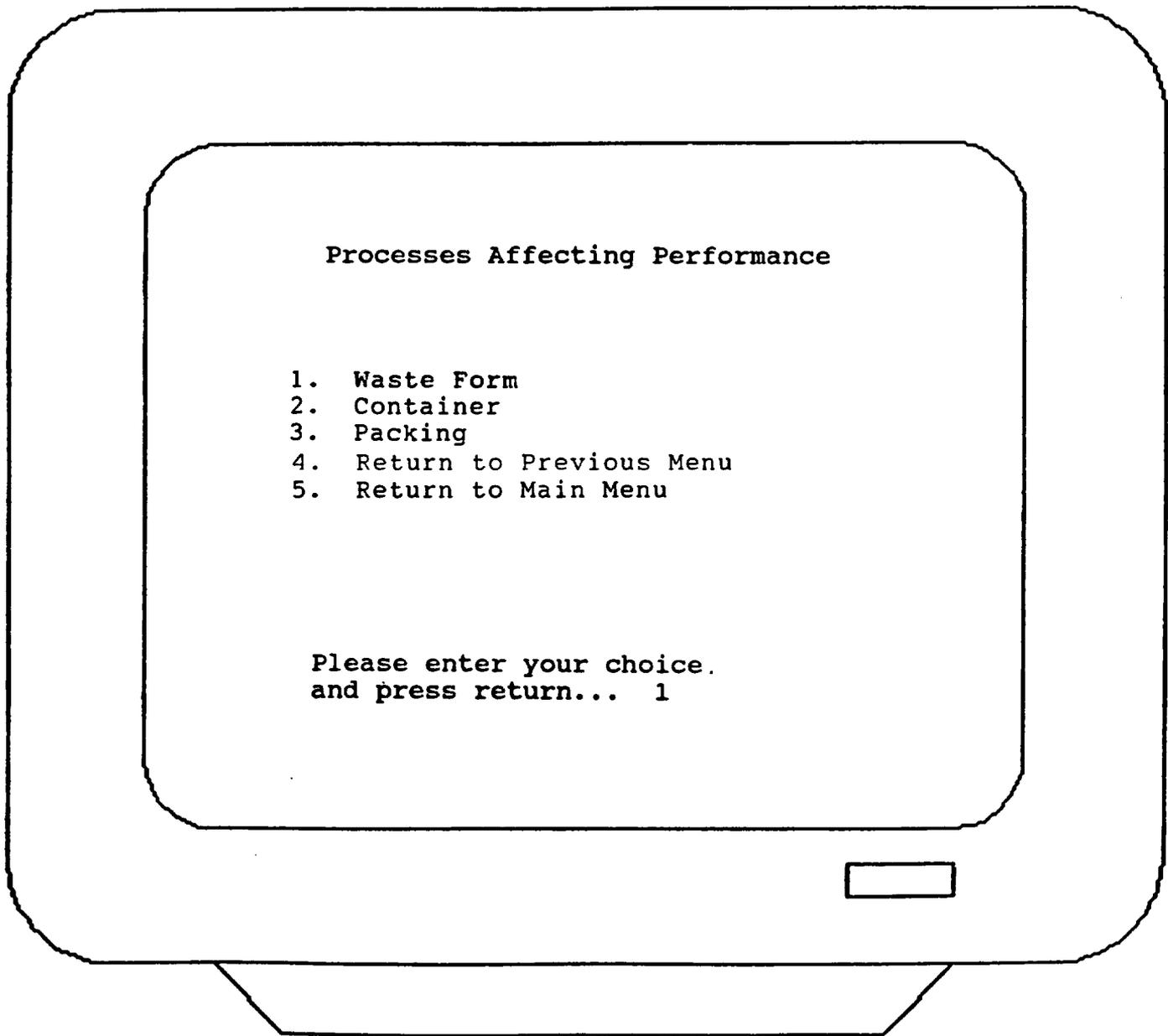


Figure 3.9. Sample LAMTRAX Parameters Menu

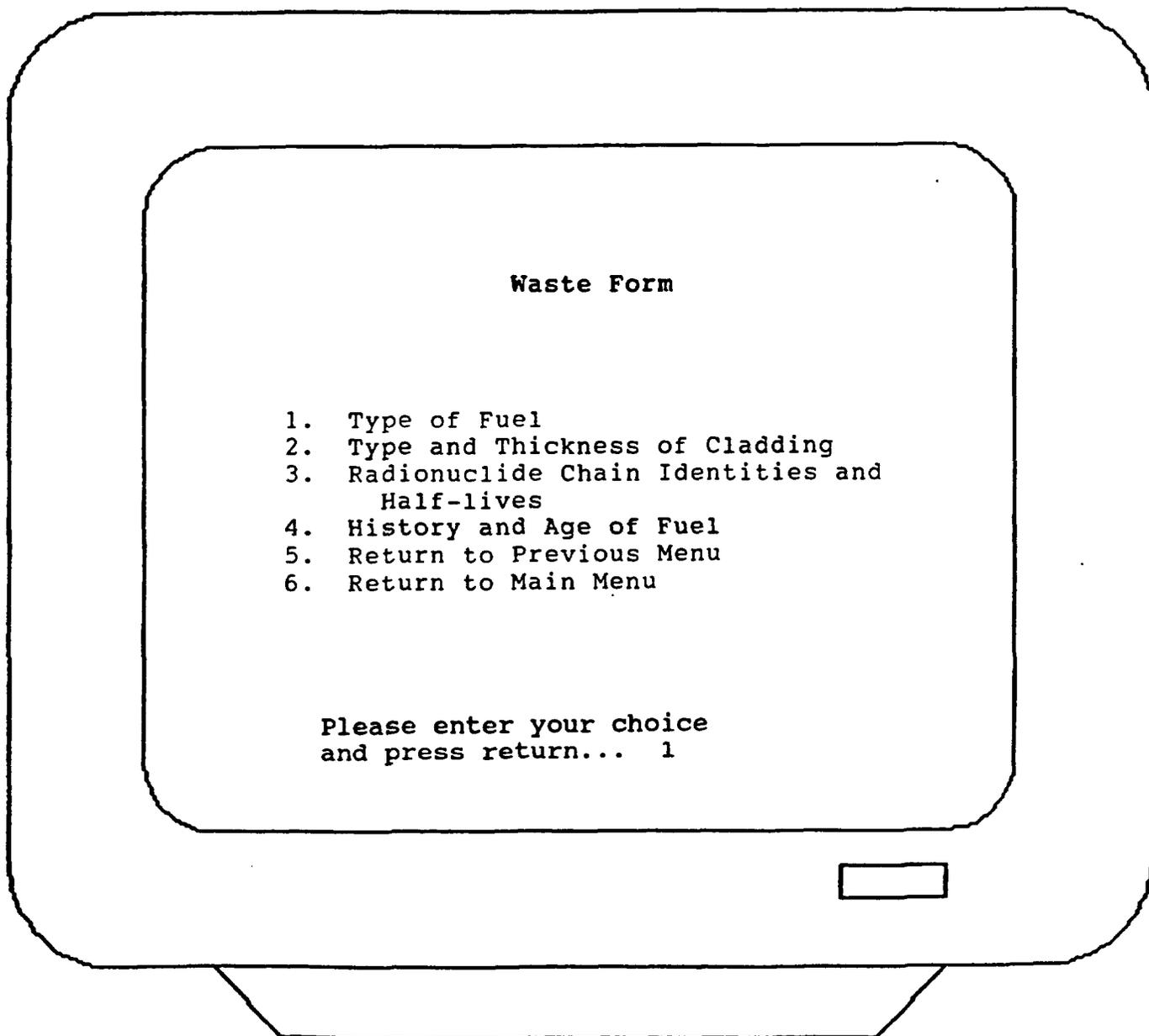
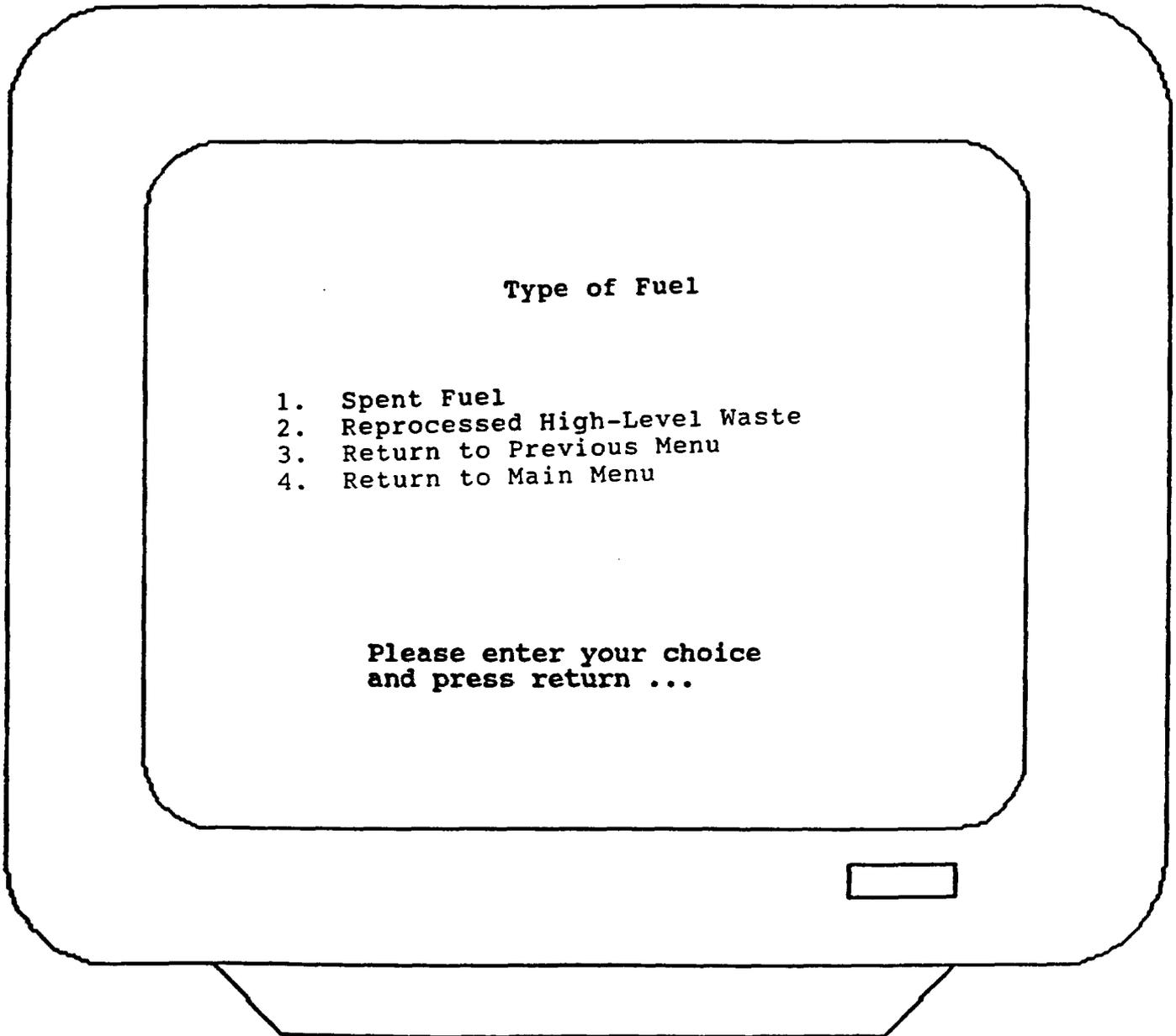


Figure 3.10. Sample LAMTRAX Waste Form Menu



**Figure 3.11. Sample LAMTRAX Fuel Type Menu**

NUREG/CR report. This document will provide the user with some history of the LAM, a reference to this report and other supporting material, some example query sessions, procedures for editing existing information if necessary, and instructions for initially installing LAMTRAX onto the user's computer from a diskette provided by Sandia. In addition, the structures of the individual databases will be described in case the need arises for future modifications. This installation diskette will contain all of the databases and the software developed by Sandia to drive the computerized system, but will not contain proprietary software such as DOS and dBASE III Plus. Finally, whenever possible, other existing databases such as the Nuclear Energy Agency Data Bank will be investigated to provide guidance and data for LAMTRAX.

Table 3.1.  
Sample Outline of the Licensing Assessment  
Methodology Tracking System (LAMTRAX)

- 1.0 Banner
- 1.1 Credits
- 1.2 Disclaimer
- 1.3 Description of System
- 2.0 Main Menu - Assessing Compliance with the Regulations
- 2.1 NRC Requirements (10 CFR Part 60.113)
  - 2.1.1 Waste Package
    - 2.1.1.1 Definition/description
      - 2.1.1.1.1 "Waste Package" means the waste form and any containers, shielding, packing, and other absorbent materials immediately surrounding an individual waste container (10 CFR Part 60.2).
      - 2.1.1.1.2 Processes That Affect Performance of WP
        - 2.1.1.1.2.1 Waste form
          - 2.1.1.1.2.1.1 Type of fuel
            - 2.1.1.1.2.1.1.1 Spent fuel
              - 2.1.1.1.2.1.1.1.1 BWR or PWR
                - 2.1.1.1.2.1.1.1.1.1 Consolidated or unconsolidated
              - 2.1.1.1.2.1.1.1.2 Reprocessed HLW
            - 2.1.1.1.2.1.1.2 Type and thickness of cladding
            - 2.1.1.1.2.1.1.3 Radionuclide chain identities and half-lives
            - 2.1.1.1.2.1.1.4 History and age of fuel
          - 2.1.1.1.2.1.2 Container
            - 2.1.1.1.2.2.1 Mechanical/Structural integrity
              - 2.1.1.1.2.2.1.1 Strength and elastic moduli
              - 2.1.1.1.2.2.1.2 Fracture toughness
              - 2.1.1.1.2.2.1.3 Thermal output
              - 2.1.1.1.2.2.1.4 Failure modes
            - 2.1.1.1.2.2.2 Corrosion properties
              - 2.1.1.1.2.2.2.1 Uniform corrosion
              - 2.1.1.1.2.2.2.2 Pitting
              - 2.1.1.1.2.2.2.3 Intergranular Stress-Corrosion Cracking (IGSCC)
              - 2.1.1.1.2.2.2.4 Radiolysis
          - 2.1.1.1.2.1.3 Packing
            - 2.1.1.1.2.3.1 Type of material
              - 2.1.1.1.2.3.1.1 Thickness
              - 2.1.1.1.2.3.1.2 Sorbing properties
        - 2.1.1.1.3 Codes
          - 2.1.1.1.3.1 Code 1

- 2.1.1.3.1.1 Description of the code
- 2.1.1.3.1.2 Applicable models already run on the code
- 2.1.1.3.1.3 References
- 2.1.1.3.2 Code 2 ...

## 2.1.2 Release Rates from Engineered Barrier Systems

- 2.1.2.1 Definition/description
  - 2.1.2.1.1 "Engineered Barrier System" means the waste package and the underground facility (10 CFR Part 60.2).
- 2.1.2.2 Parameters affecting performance
  - 2.1.2.2.1 Transport through waste package (see "Waste Package")
    - 2.1.2.2.2 Transport through Engineered Barrier System
      - 2.1.2.2.2.1 Flow parameters
        - 2.1.2.2.2.1.1 Boundary conditions
        - 2.1.2.2.2.1.2 Other parameters (see "Ground-water Travel Time")
          - 2.1.2.2.2.2 Coupled heat and mass transport
            - 2.1.2.2.2.2.1 Heat source term
            - 2.1.2.2.2.2.2 Thermal properties of waste package
              - 2.1.2.2.2.2.2.1 Density
              - 2.1.2.2.2.2.2.2 Conductivity
              - 2.1.2.2.2.2.2.3 Specific heat (heat capacity)
              - 2.1.2.2.2.2.2.4 Surface emittance
            - 2.1.2.2.2.2.3 Transport through each layer of the waste package
              - 2.1.2.2.2.2.3.1 Waste form (see "Waste Package")
              - 2.1.2.2.2.2.3.2 Packing (see "Waste Package")
              - 2.1.2.2.2.2.3.3 Backfill (see "Waste Package, Packing")
  - 2.1.2.2.2.3 Codes (see "Waste Package")

## 2.1.3 Ground-water Travel Time

- 2.1.3.1 Definition/description
  - 2.1.3.1.1 The travel time of a particle of water along the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment. Minimum acceptable time is 1000 yrs (10 CFR Part 60.113).
- 2.1.3.2 Parameters affecting performance
  - 2.1.3.2.1 Hydrologic factors
    - 2.1.3.2.1.1 Hydraulic conductivity
    - 2.1.3.2.1.2 Effective porosity
    - 2.1.3.2.1.2 Hydraulic gradient
    - 2.1.3.2.1.3 Fluid density
    - 2.1.3.2.1.4 Other factors
  - 2.1.3.2.2 Geologic factors
    - 2.1.3.2.2.1 Rock Type
    - 2.1.3.2.2.2 Degree of fracturing
      - 2.1.3.2.2.2.1 Orientation
      - 2.1.3.2.2.2.2 Location
      - 2.1.3.2.2.2.3 Aperture
      - 2.1.3.2.2.2.4 Porosity
    - 2.1.3.2.2.3 Thickness of formation
  - 2.1.3.2.3 Geochemical factors
    - 2.1.3.2.3.1 pH/Eh

- 2.1.3.2.3.2 Kd/retardation
- 2.1.3.2.3.3 Chemical composition of host rock
- 2.1.3.2.3.4 Other factors
- 2.1.3.2.4 Natural processes/scenarios
  - 2.1.3.2.4.1 Volcanism
  - 2.1.3.2.4.2 Seismicity
  - 2.1.3.2.4.3 Subsidence
  - 2.1.3.2.4.4 Dissolution
  - 2.1.3.2.4.5 Flooding
  - 2.1.3.2.4.6 Glaciation
  - 2.1.3.2.4.7 Extreme erosion
- 2.1.3.2.5 Sensitivity/Uncertainty Analysis
  - 2.1.3.2.5.1 Spatial variation
  - 2.1.3.2.5.2 Temporal variation
- 2.1.3.2.6 Possible future rule changes
- 2.1.3.3 Codes (see "Waste Package")

## 2.2 EPA Requirements (40 CFR Part 191 and 10 CFR Part 60.112)

### 2.2.1 Containment Requirements (40 CFR Part 191.13)

#### 2.2.1.1 Definition/Description

- 2.2.1.1.1 Release limits apply to the accessible environment.
- 2.2.1.1.2 Release limits apply to first 10,000 years post closure.
- 2.2.1.1.3 Controlled Area shall not extend more than 5 km from edge of repository and shall not exceed 100 km<sup>2</sup>.
- 2.2.1.1.4 Release limits computed in 40 CFR Part 191-Appendix A apply to release levels expected to occur with a cumulative probability of greater than 0.1 over the 10,000 year period.
- 2.2.1.1.5 Those same release limits, if increased by one order of magnitude, apply to release levels expected to occur with a cumulative probability of greater 0.001 over the 10,000 year period.
- 2.2.1.1.6 No limits are placed on release levels expected to occur with a cumulative probability of less than 0.001 over the 10,000 year period.
- 2.2.1.2 Processes that affect overall system performance
- 2.2.1.3 Relevant phenomena and parameters
- 2.2.1.4 Codes (see "Waste Package")

### 2.2.2 Groundwater Protection Requirements (40 CFR Part 191.16)

#### 2.2.2.1 Definition/Description

- 2.2.2.1.1 Apply to first 1000 years post-closure
- 2.2.2.1.2 Apply to Class I ground waters that are:
  - 2.2.2.1.2.1 within the controlled area or less than 5 km beyond the controlled area,
  - 2.2.2.1.2.2 supplying drinking water for thousands of persons as of the date that the site is selected as a potential repository,
  - 2.2.2.1.2.3 irreplaceable in that no reasonable alternative source of drinking water is available.
- 2.2.2.1.3 Radionuclide concentrations shall not exceed those

- established for community water systems in 40CFR141.
- 2.2.2.2 Processes That should be considered when predicting concentrations of radioactive elements in ground water.
  - 2.2.2.3 Relevant phenomena and parameters.
  - 2.2.2.4 Codes (see "Waste Package")
- 2.2.3 Individual Protection Requirements (40 CFR Part 191.15)
- 2.2.3.1 Apply to first 1000 years post-closure.
  - 2.2.3.2 Annual shall be no more than 25 millirems to the whole body or 75 millirems to any organs.
  - 2.2.3.3 This exposure limit assumes ingestion of 2 liters per day of water from a "significant source" of groundwater outside the controlled area.
  - 2.2.3.4 A "significant source" is one that:
    - 2.2.3.3.1 is saturated with water containing less than 10,000 mg per liter of total dissolved solids,
    - 2.2.3.3.2 is within 2500 ft. (762 m) of the land surface.
    - 2.2.3.3.3 has a transmissivity of at least 200 gallons per day per foot ( $2.9E-05 \text{ m}^2/\text{s}$ ) provided that,
    - 2.2.3.3.4 each of the underground formations or parts of the underground formations included within the aquifer must have a hydraulic conductivity greater than 2 gallons per day per square foot ( $9.4E-07 \text{ m/s}$ ), and
    - 2.2.3.3.5 must be capable of providing a sustained yield of 10,000 gallons per day ( $4.4E-04 \text{ m}^3/\text{s}$ ) of water to a pumped or flowing well.
  - 2.2.3.5 Codes (see "Waste Package")
- 2.3 Quit

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