Evaluation of a Performance Assessment Methodology for Low-Level Radioactive Waste Disposal Facilities

Validation Needs

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Abstract

In this report, concepts on how validation fits into the scheme of developing confidence in performance assessments are introduced. A general framework for validation and confidence building in regulatory decision making is provided. It is found that traditional validation studies have a very limited role in developing site-specific confidence in performance assessments. Indeed, validation studies are shown to have a role only in the context that their results can narrow the scope of initial

investigations that should be considered in a performance assessment.

In addition, validation needs for performance assessment of low-level waste disposal facilities are discussed, and potential approaches to address those needs are suggested. These areas of topical research are ranked in order of importance based on relevance to a performance assessment and likelihood of success.

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FOREWORD

This technical contractor report is a product of Sandia National Laboratories under project FIN L1153. The purpose of this program is to update and improve a performance assessment methodology for low-level radioactive waste disposal facilities previously developed under FIN A1764.

NUREG/CR-5927 is not a substitute for NRC regulations and compliance is not required. The approaches and/or methods described in this NUREG/CR are provided for information only. Publication of this report does not necessarily constitute NRC approval or agreement with the information contained herein.

1.0 Introduction

1.1 Background

Sandia National Laboratories (SNL) has been contracted by the U.S. Nuclear Regulatory Commission (NRC) to develop a performance assessment methodology to evaluate disposal sites containing low-level radioactive waste. The purpose of the methodology is to allow NRC to conduct confirmatory analyses of a licensee's evaluation of postclosure impacts at a low-level waste disposal site. The evaluation must provide reasonable assurance that the performance objectives in 10 CFR Part 61.41 are met.

Initially, a generic pathway analysis was conducted for shallow land burial [Shipers, 1989]; based on this analysis, Shipers and Harlan [1989] identified the two most important pathways. These two pathways consisted of (1) the pathway from the source, through ground water, to a water well, with subsequent exposure of humans through contaminated well water, and (2) the pathway from the source, to ground water, to surface water, with subsequent exposure of humans and foodstuffs through contaminated surface water. More recently, Rao *et al.* [1992] conducted a pathway analysis for disposal technologies other than shallow-land burial, and also concluded that the well-water pathway was the most significant. The assessments were performed for generic sites, and it is possible that at specific sites the well-water pathway may not be the most significant. For example, if the site is located over an aquifer that is very saline (and unpotable), the well-water pathway may not be the most significant pathway (e.g., Baird *et al.*, 1990). However, it is expected that these cases will be rare, and that the well-water pathway will dominate the exposure pathways in most cases.

Based on the pathways identified by Shipers and Harlan [1989], Kozak *et al.* [1989] identified several distinct modeling needs for performance assessment of low-level waste disposal facilities. These areas consisted of source-term release, ground-water flow and transport, air transport, surface-water transport, food-chain transport, and dosimetry. Models for each area were identified or developed, and integrated into a methodology. This system of integrated models, implemented in the form of computer codes, is what is referred to as the low-level waste performance assessment methodology [Kozak *et al.*, 1990a].

One of the requirements for the methodology was that it must be flexible enough to handle a wide range of potential low-level waste disposal sites. Based on this requirement, the performance assessment modeling needs

to range from very simple to somewhat more complex, and models are included in the methodology for both of these purposes. However, the underlying philosophy was to emphasize reasonably conservative, simple analyses. This was because the methodology was developed for assessing analyses and assumptions in a licensee's application. However, there is a clear need to be able to model either portions of the system or the whole system, as necessary.

The update of the methodology's modeling capabilities, published in Volume 1 of this report [Kozak *et al.*, 1993], expanded and improved these capabilities. Greater attention was placed on global issues such as uncertainty analysis and the manner in which site-specific data should be used in supporting a defensible regulatory decision. SNL was also assigned the task of evaluating the validation needs of the methodology. Consequently, SNL has continued to develop conceptual approaches related to validation: what it is, what it intends to accomplish, and how it is to be used. This report will address validation issues related to low-level waste performance assessment. Issues are addressed that range from the general to the specific. It describes a framework in which validation studies may have a positive effect on decision making through performance assessments, and defines which areas of the low-level performance assessment methodology are best addressed by this framework. Furthermore, it (1) introduces concepts on how validation fits into the scheme of developing confidence in performance assessments, (2) identifies the validation needs for the low-level waste performance assessment methodology [Kozak *et al.*, 1990b; Kozak *et al.*, 1993], (3) identifies potential approaches to address those needs, and (4) ranks the validation needs in order of importance, based on relevance to a performance assessment and likelihood of success.

1.2 Scope

In Chapter 2, recent advances in the understanding of validation of performance assessment models are reviewed, and their implications for the performance assessment process are described. New concepts are introduced on the role of validation studies in the overall scheme of developing performance assessment confidence. These concepts are generally applicable to all performance assessments, whether they are conducted for near-surface, above-ground, or deep geological disposal facilities. In Chapter 3, these concepts are applied to models needed for low-level waste performance assessment. Since these models represent the general needs of performance

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assessment modeling for land disposal facilities, Chapter 3 is also broadly applicable, and is not intended to be

limited to the current NRC/SNL performance assessment methodology.

2.0 A Framework for Performance Assessment, Validation, and Confidence

2.1 Developments in Ideas on Validation

In the past few years, the waste management community has seen a marked shift in concepts related to validation of performance assessment models. In this section, we review this shift in ideas, outline the current consensus (as far as it exists) about validation, and provide suggestions on the role of validation in performance assessment. We acknowledge beforehand that validation remains a contentious topic, and that not all readers will agree with the positions stated in this section.

There have been many studies that have investigated model validation as it pertains to performance assessment of waste disposal sites. Most notable among validation programs for ground-water flow and transport have been INTRACON [1986], HYDROCON [1990], and INTRAVAL [1990]. These programs represent a long evolution of thought about what validation means and what its role in the regulatory process should be. Much of the philosophical debate about validation has taken place during meetings of these programs. At the completion of the most recent of these programs (INTRAVAL Phase 2), a striking conclusion was reached:

Model validation, in its usual scientific sense, is unachievable for performance assessment models.

The main issue leading to this conclusion is that the functional capabilities of performance assessment models cannot be observed or evaluated over the time frames or the space scales at which they will be applied [Davis *et al.*, 1991]. That is, the fundamental principle of science is violated: the scientist must be able to empirically observe the phenomenon of interest in order to confirm or revise ideas about it.

The problems involved in performing performance assessment validation reduce to the following.

- (1) Analyses involving geological systems are invariably dominated by geometrical effects at all scales (boundaries, spatial structure, spatial heterogeneity). These geometrical considerations are *always* a unique site-specific combination. This means that performing analyses of one site produces information that is unique to that site. Transfer of such information from one site to another is a dubious approach at best. Validation of models of geological systems is therefore

reduced to an activity that is indistinguishable from site-specific characterization.

- (2) Performance assessments must invariably evaluate conditions that cannot be observed. The only climatic conditions that can be observed are those existing today, a brief snapshot in a long-term waste repository. Studies done prior to construction of the disposal facility cannot account for the influence of the facility on the system. Full system validation studies can never be carried out from source to dose, so large portions of the model must remain unstudied.
- (3) Performance assessment must be carried out over such large time and space scales that the phenomena of interest cannot be observed, even for current conditions. This means that the scientific method (make a hypothesis, observe the system behavior, and use those observations to modify the hypothesis) cannot be used for performance assessment. Natural analogue studies, which have the potential for spanning the appropriate time and space scales, are generally too complex to be matched by the relatively simple models used for performance assessments. Furthermore, the initial condition of natural analogues is universally unknown, which makes the problem of matching data to models nonunique.
- (4) Performance assessment data on geological systems are so sparse that unambiguous answers are virtually impossible to achieve [Davis and Goodrich, 1990; Davis *et al.*, 1991]. Since the data are so sparse, numerous competing conceptual models can be proposed and supported.

This lack of ability to conduct meaningful validation studies on performance assessment models has profound consequences for all aspects of performance assessment. Concepts about the meaning and significance of validation have been subdivided into the teachings of adherents of two differing camps. Adherents of the first camp hold that performance assessments should be rooted in a realistic estimate of the expected behavior of the facility. Reasonable assurance, in this view, is based on scientifically understanding the site, then allowing an additional margin of safety outside of the expected uncertainty in the outcome [National Research Council, 1990; Wierenga *et al.*, 1993]. This concept is depicted in Figure 1. Adherents of the second philosophical camp on

Figure 1 The concept of the goal of performance assessment according to the first philosophical camp. Adapted from the concept described in National Research Council [1990], p. 278.

performance assessment hold that realistic performance can never be known with confidence, and that reasonable assurance is demonstrated by beginning with bounding conservatism, and reducing that conservatism to the extent necessary and to the extent it is defensible [Davis *et al.*, 1991]. In this view, reasonable assurance is produced because the uncertainty all lies toward the direction of greater safety, as shown in Figure 2. In our opinion, the conclusions of the INTRAVAL group are consistent with this second philosophy. They support the notion that a realistic result can never be known with confidence. Consequently, there cannot be any confident basis for defining reasonable assurance in terms of the magnitude of departure from reality; that magnitude will never be known with confidence.

In our view, performance assessments cannot be thought of as scientific demonstrations of the safety of a site, since the scientific method cannot be used. Furthermore, the goal of performance assessments cannot be thought to be prediction or accurate estimation of consequences resulting from the disposal, since we cannot judge the accuracy or predictability of the models [Pigford, 1992]. In fact, the few studies that have conducted postaudits of the

long-term predictability of contaminant transport have shown generally bad correspondence between predicted and measured contaminant concentrations [Robertson, 1974; Konikow, 1986; National Research Council, 1990; Bredehoeft and Konikow, 1993]. That is, current site-specific models have been shown to be quite inaccurate, even for relatively short-duration predictions. Based on these views, performance assessment begins to appear markedly different from nuclear reactor probabilistic risk assessment (PRA), to which it superficially appears quite similar. PRA models can be compared with real-world examples, in which the entire system is examined over the duration of its lifetime. Consequently, information about expected failure rates of components can be revised over a period of time. The link between empirical observation and model improvement is retained in PRA. By contrast, performance assessment models will never be tested for an entire system, or for the time periods of importance. Performance assessment modelers will never have the opportunity to learn from their failures.

All of this suggests that performance assessment modelers must use fundamentally different mechanisms for developing confidence in their models. We have argued

Figure 2 Reasonable assurance according to the second philosophical camp.

elsewhere [Kozak, in press; Kozak *et al.*, 1993] that in the context of performance assessment, the concept of validation of performance assessment models may be replaced by the concept of confidence in the regulatory decision. Comfortable regulatory decisions can be made in the absence of scientific confidence, because the problem is not a scientific one. For instance, a clearly conservative model is acceptable for regulatory decisions even though it is inaccurate (a conservative model must by nature be inaccurate), and hence scientifically unacceptable. Science puts rational constraints on the believability of the model, but is not the purpose of the model. Regulatory confidence comes from a believable conservative bias rather than from any notion of accuracy [Pigford, 1992]. Indeed, the regulatory problem is to solve an inequality (the dose must be less than...), which is an intrinsically much simpler problem than attempting accuracy.

Therefore, a clear distinction must be made between *scientific* confidence and *regulatory* confidence. Scientific confidence is impossible to achieve for analyses stretching over many thousands of years. On the other hand,

regulatory confidence *can* be achieved. It is critically important to realize that regulatory confidence is achieved by different mechanisms than is scientific confidence, and that scientific confidence plays an important, but small, role in developing regulatory confidence. This role has not heretofore been clearly defined; in the following section, we attempt such a definition.

2.2 The Role of Validation in Developing Confidence

The process of performance assessment, as has been previously discussed [Kozak *et al.*, 1993], begins with an initial assessment of currently available data, as shown in Figure 3. Assumptions developed from the initial database need to be as broad as possible, since one cannot in general identify which assumptions are conservative relative to other assumptions. Implicit in this approach is that we are seeking a conservatively biased analysis that lends itself to providing regulatory confidence. The analyst is not seeking an *accurate* answer, but rather a *range* of possible answers that adequately represent the current level of uncertainty.

Figure 3 The process of performance assessment described by Kozak *et al.* [1993].

When site-specific data are unavailable for developing assumptions about a model, or for assigning a range to parameter distributions used in the modeling, very broad ranges must be used. For instance, if site-specific data are unavailable for a particular parameter, the range might be determined from the widest set of values ever measured. These assumed values would have a generic nature, since they would provide a common starting place for all performance assessments. In this way, generic (literature) information can be incorporated into the performance assessment as an initial assumption set. Of course, this initial assumption set may also be chosen to be more site specific if the initially available data set supports the assumptions.

Continuing through the process shown in Figure 3, the initially assumed values are propagated through a suite of models to arrive at consequences (doses) for each model

and parameter realization. (The simultaneous treatment of model and parameter uncertainties is discussed at greater length in Kozak *et al.* [1991], Davis and Olague [1991], and Kozak *et al.* [1993].)

The significance of using assumed values in this manner is that the data only need to be site-specific if they influence the results of the performance assessment. If one used assumed values for, say, the sorption coefficient, K_d , of Co-60, and if the consequence analysis using conservative modeling demonstrated negligible dose from Co-60, then Co-60 K_d data need never be collected. On the other hand, if we discover after the first performance assessment iteration that the Co-60 K_d is an important parameter, this suggests that greater attention should be paid to justifying the values used in the assessment. Here an important parameter is defined as one that is both uncertain and leads to noncompliance. In this case, the

facility does not meet the performance objectives because of the broad assumed distribution assigned to this parameter, and there is an incentive to make the distribution narrower. This can be accomplished by acquiring more site-specific data, which can be used in subsequent performance assessment iterations.

The process can therefore be thought of as a progression from the generic to the specific, from assumed values to measured ones, and from broad parameter ranges and assumptions to progressively narrower conditions, as shown in Figure 4. In an ideal physical setting, the potential exists for using only assumed ranges for many parameters of interest, and to demonstrate compliance without taking any site-specific data on many parameters of interest. Of course, this approach is only appropriate if the initial range applied in the modeling is sufficiently broad. The iterative process is necessarily site-specific, and revolves around gathering and using site-specific data.

The role of generic validation studies in this scheme is, at best, limited.

However, validation can play an auxiliary role in making this process more efficient and defensible. Earlier, we have pointed out that validation is an inappropriate concept for developing confidence in performance assessments. However, the performance assessment procedure begins with an envelope of extant knowledge about possible models and parameter ranges. It is to this knowledge base that validation studies should be addressed. It is important to realize that in the performance assessment strategy, the breadth of the "knowledge envelope" for a property is inversely related to the breadth of the parameter distribution or suite of models that represents our uncertainty about that property. That is, if we know nothing about a property of the system, we must permit it to vary widely, to encompass our (complete) uncertainty. This breadth is then

Figure 4 Progression of the information used in performance assessment from generic to specific as iterations proceed.

Framework

progressively reduced as the assessment process progresses, and as it is determined which information is needed to demonstrate compliance.

Validation studies can be envisioned that are directed either toward expanding the current knowledge envelope, or toward contracting it. Validation studies aimed at expanding the envelope would look for aberrant or unusual conditions that would call current modeling paradigms into question. That is, these studies would be directed toward finding conditions that we do not currently know exist, and which would tend to make current models nonconservative. Clearly, this is an extraordinarily difficult task, for there is no established scientific mechanism for conducting such studies. "Normal" science is concerned with providing adequate descriptions of known phenomena, not with searching for unknown phenomena [Kuhn, 1970]. The other goal for validation studies, that of shrinking the current uncertainty envelope within established paradigms, can be addressed using the scientific method, and is both achievable and desirable. The rationale for such studies would be to reduce the breadth (hence conservatism) with which all performance assessments should start. That is, by incorporating as many assumptions as possible, using wide parameter distributions, one attempts the difficult task of guessing the conservative conditions beforehand. However, the goal, from the standpoint of efficiency, is to narrow the conditions to the extent possible. This type of validation study is particularly appropriate for conditions and properties that have not been studied to a great degree, so that the knowledge envelope associated with them is small, and distributions describing them are large. However, these validation studies must still be closely linked to the modeling needs of performance assessments. Clearly, in order to build confidence in performance assessments, the phenomena studied must be pertinent and important to the assessment.

The process of building confidence in a performance assessment is therefore seen to be entirely a site-specific exercise. Confidence that the site will indeed comply with performance measures is produced by a consistent conservative bias, with conservative assumptions removed as needed through progressive iterations of the assessment.

Owing to this approach, the calculations used for assessing compliance may have relatively small resemblance to conditions existing at the site. In using this approach, validation studies seeking to obtain accurate descriptions of phenomena of interest can influence the process only by altering its initial conditions. Validation studies can improve the understanding of some conditions known to be important in a generic way to the performance assessment, and in this manner make all performance assessments more efficient (by narrowing the set of initial conditions that must be considered). Alternatively, they can uncover aberrant conditions that would open new areas of concern. Only the former of these two approaches can be addressed in a systematic manner.

2.3 Validation and Low-Level Waste Performance Assessment

The remainder of this report is devoted to identifying particular areas in land disposal performance assessments that may benefit from these kinds of validation studies. In each portion of the performance assessment methodology, areas are identified in which the current knowledge base is narrow (that is, little is known about the subject), which would then suggest that broad initial modeling assumptions need to be applied at all sites. Our goal is to identify areas that, if adequately resolved, might broadly affect all performance assessments by narrowing the set of conditions that need to be considered.

In evaluating the relative importance of addressing validation issues, two principal criteria have been applied. First, the issue must be important to performance assessment in a generic way. Second, there must be good potential for successfully influencing performance assessments in a generic way. These two criteria have been applied to the broad categories of performance assessment models. For the purposes of this report, these subdivisions are the behavior of the disposal facility, the hydrosphere, the atmosphere, and the biosphere. The disposal facility is further subdivided into assessments related to flow through the disposal units, and issues related to the chemical behavior of the system.

3.0 Validation Related to Component Models of the Performance Assessment

In the following sections, models that are used to simulate each major component of the methodology are discussed, and important assumptions associated with each model are identified, along with potential validation cases that may be able to test those assumptions. In addition to comparisons with experimental observations, modeling studies are also recommended to develop improved understanding of processes of concern. Such studies must be viewed as a first step in developing confidence in the portion of the analysis to which they are directed. To provide true confidence, modeling studies must be backed up by experimental information. However, in some cases such data are unavailable, and modeling studies are recommended as an interim step in developing adequate confidence.

3.1 The Disposal Facility

In low-level waste performance assessment, the source term is defined as the time-dependent rate of radionuclide release from the boundary of the facility's disposal units [Kozak *et al.*, 1990b]. To estimate this release rate, several different component models are required. These include models of gas generation, the flux of ground water into the disposal system, barrier degradation, leaching, and ground-water flow and transport within the disposal facility. Models that are used for each of these areas are discussed in the following sections.

3.1.1 Gas Generation

Potential gaseous radionuclides in low-level waste include ^3H , ^{14}C , ^{85}Kr , and ^{222}Rn . In general, gas generation of ^{14}C is probably most important because of its relatively long half-life; therefore, the following discussion concentrates on gas generation of ^{14}C . However, it should be noted that, although radon's half-life is relatively short, it is the parent of long-lived species. Furthermore, the possibility exists for gaseous transport of radon to plant roots, and then decay of radon to longer lived radionuclides. This could produce a significant dose to man if bioaccumulation in edible plant roots occurs. Currently, studies investigating this possible exposure pathway are unknown to us. Gas-phase transport of ^{85}Kr and ^3H will be unimportant except perhaps during the period of institutional control, since both radionuclides have short half-lives and decay to stable isotopes.

The methodology does not currently contain a method for estimating the rate, volume, or radiological component of gas production from low-level waste in a disposal facility. As this is an area where there has been relatively little

research, data are unavailable to justify the use of any model at the present time. The studies that exist on gas generation that exist (e.g., Matuszek and Robinson, 1983; Matuszek, 1988) represent different chemical conditions than are expected in future vault designs. Any performance assessment model used to calculate potential gaseous releases can currently only be justified by using arguments about conservatism. Most existing approaches to modeling gas generation have been developed for different inventories than U.S. low-level waste streams (e.g., Biddle *et al.*, 1987). Recently, there has been an effort to develop a better understanding of the mechanisms of release of gaseous ^{14}C , and this work is expected to produce the framework for understanding that is needed for performance assessment [Yim *et al.*, 1993]. Preliminary work appears to demonstrate that the release of ^{14}C in the gas phase may be rate-limited by the access of water to the waste.

Gas generation may be important for low-level waste performance assessment because of the following considerations.

- (1) Releases into the gas phase may decrease the impacts of the ground-water pathway. For some low-level waste inventories, ^{14}C doses can make a substantial contribution to the ground-water dose. The doses from the air pathway and the ground-water pathway are likely to occur at very different times, so the peak dose to the maximally exposed person from the ground-water pathway may potentially be reduced by accounting for gas releases.
- (2) The potential exists for bioaccumulation of gaseous $^{14}\text{CO}_2$ in plants. This could concentrate otherwise unimportant releases in the gas phase. Consequently, this mechanism poses a possible enhanced transport path from the disposal cells.
- (3) The aforementioned possibility of radon transport may provide a preferential pathway for some of its progeny.

Gas generation models are intricately linked to assumptions about conditions that exist inside the low-level waste disposal facility for the performance assessment time period. Conditions inside the disposal facility have large uncertainties associated with them because of the heterogeneous nature of low-level radioactive waste. These uncertainties can be reduced to some extent for stabilized waste forms.

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For gas production models, the mechanisms assumed to be occurring are (1) microbial biodegradation of organic materials, leading to releases of $^{14}\text{CO}_2$ and $^{14}\text{CH}_4$, (2) production of tritiated H_2 gas from metal corrosion, and (3) ingrowth of gaseous radioactive progeny, such as ^{222}Rn . The most important validation issue associated with ^{14}C gas generation models is the need to determine whether microbial conversion to gaseous ^{14}C is a significant process [Jefferies, 1990], and if it is important, to determine a rate of production of the gas. The desire is to produce bounding estimates of the potential rate of gaseous production of ^{14}C for use in the performance assessment. However, one cannot make a general statement that an assumption of high rates of production of gaseous ^{14}C is conservative, since the carbon may partition between gas and ground-water pathways. High rates of gas production may potentially decrease ground-water impacts. Consequently, a range of potential gas release rates must be examined to determine which assumptions are conservative with respect to the complete analysis. The rate of gas production is expected to depend on (1) the effect of relatively high pH porewaters (characteristic of cementitious environments) on microbial biodegradation, and (2) whether the nutritional requirements of the bacteria are met in a low-level waste disposal facility. These nutritional requirements are dependent upon both inventory and facility design considerations.

Models for the release of radionuclides into the gas pathway have two primary components: gas production and subsurface transport. Yim *et al.* [1993] have suggested that in many current vault designs, transport will be dominated by access standpipes and drainage systems. Transport in such systems will be essentially instantaneous compared with the half lives of any of the gaseous radionuclides. Furthermore, transport through standpipes will not dilute or disperse the gases to any significant extent. Consequently, subsurface transport is not expected to be a fruitful area of research to examine for reducing conservatism.

A validation test case for gas generation models would consist of comparing currently available gas generation models to measurements from U.S. low-level waste under the physical and chemical conditions likely to be encountered by the waste in a disposal unit. Since most current disposal designs include massive use of concrete, the experiment should be conducted for high pH. Such an experiment would also be appropriate for many arid western sites, which are the only ones for which trench burial is currently being considered. The experiment

should be conducted over relatively large spatial and temporal scales, which would likely require a substantial investment in time and resources. However, accelerated tests are unlikely to provide meaningful results, since the gas production mechanism of greatest interest, microbial biodegradation, is not amenable to accelerated testing. At present, we are unaware of any suitable experimental data sets that could be used in a test case for validation of gas generation models.

Gaseous releases from low-level waste disposal facilities tend to be unimportant relative to the ground-water pathway. Consequently, research directed toward gas-phase release and transport will have a low impact on performance assessment capabilities. Furthermore, any experiment on gas production rates will be limited in the amount of general information it produces, since gas generation will be strongly influenced by site-specific, design-specific, and inventory-specific conditions. Consequently, this area of research can be rated as both low impact and low likelihood of providing general information.

3.1.2 Barrier Degradation

There are several kinds of man-made barriers in facility designs for low-level waste disposal: concrete structures, steel containers, and engineered soil barriers. These barriers serve two functions: they provide structural stability, which minimizes subsidence, and they exhibit low permeability to water, minimizing contact of water with the waste. With proper engineering design, it is generally believed that low-level waste disposal facilities can be built that will structurally withstand the forces on them for very long periods. The permeability of barriers is another matter. Assuming adequate structural stability, the behavior of the barriers over lifetime of the disposal facility translates into the following stages: (1) intact (low permeability), (2) partially degraded (moderate permeability), and (3) failed (high permeability). The duration of these stages and the absolute magnitude of the effective permeability of the barrier are the key pieces of information needed in a performance assessment.

The intact stage of man-made barriers is important primarily to contain short-lived radionuclides (half-lives less than 100 years) within the facility. Low-level waste inventories are characterized by short-lived species and long-lived species, with few half-lives in the 50 to 1000-year range. It is clear that near-surface structures cannot be expected to function flawlessly for periods of more than a few hundred years. Consequently, the structures

cannot last long enough to contain the long-lived species until they are no longer radioactive. Nevertheless, if the intact barrier can be relied on to contain the short-lived radionuclides until they are no longer radioactive, only the long-lived radionuclides become important for performance assessment. Most studies of concrete degradation have focused on the service lifetime of concrete, with limited studies on its flow and transport behavior [Clifton and Knab, 1989; Walton *et al.*, 1990, Walton and Seitz, 1991]. All of the models for service life are designed to predict a single time at which the concrete structure fails. This failure is assumed to be an instantaneous and complete loss of functional capability, usually because of structural failure.

Many uncertainties related to concrete degradation have not been addressed, including (1) quality assurance and quality control in concrete formation, (2) extrapolation of small-scale laboratory results to the actual concrete structure, and (3) the effect of joints and potential drain obstructions (sediment or biological clogging). All of these may influence the degree to which reliance can be placed on intact performance of concrete structures.

Once a minimum intact lifetime is established, the next step is to establish a time-dependent increase in permeability for use in performance assessment. In an earlier report, we described using an assumption of a step change in permeability at some assumed time [Kozak *et al.*, 1993]. This is equivalent to an assumption that the concrete permeability "fails" instantaneously and completely. This approach was taken because there was no basis for modeling the partially degraded state of the engineered barriers, and because it is believed to be conservative under most circumstances.

Most available models have been developed to estimate a time of failure, not to model time-dependent degradation, and models that do attempt to estimate degradation have little empirical basis. Uncertainties arise because of incompletely understood degradation mechanisms [MacKenzie *et al.*, 1986]. Furthermore, there is no long-term experience with modern concrete from which to make judgments, and most experimental studies are based on short-term accelerated tests. One of the most important degradation mechanisms appears to be corrosion of the reinforcing steel used in most concrete structures. Besides these inherent uncertainties, there is also uncertainty about the future condition of the site. An important point to note is that, while the *most probable* failure mode may be some gradual failure, there may still be a chance that the failure could be rapid.

For modeling container degradation, the main mechanism assumed to occur is corrosion of metal containers. Corrosion models described by Sullivan *et al.* [1988] and Sullivan and Suen [1989] have been recommended. These models are semiempirical and produce estimates of the time and the rate of failure of containers. However, they have large uncertainties associated with them:

- (1) Specific information (e.g., soil type and moisture content in contact with the metal) about conditions inside the disposal unit is required. This information is frequently highly uncertain because of the heterogeneous nature of low-level radioactive waste. This uncertainty could be reduced through the use of specific engineering designs.
- (2) The models are based on limited data about underground corrosion [Kozak *et al.*, 1989].
- (3) The models are based on measurements of corrosion in soil, and may not be appropriate in cementitious environments.

However, it is believed that in most cases concrete structures will last longer than metallic containers, so corrosion models may be of limited importance. Consequently, the following discussion focuses on concrete degradation models.

The uncertainties identified above for concrete degradation models translate into the following validation issues (1) establishing long-term experimental studies aimed at estimating time-dependent degradation mechanisms, as opposed to service life, (2) the effects of quality assurance and quality control during formation, (3) the appropriateness of short-term accelerated tests, (4) the effects of joints and drainage systems, and (5) extrapolation of small-scale laboratory results.

To address these issues, a potential validation test case would be an analogue which uses records from cement structures (e.g., earth-mounded bunkers). Records from structures that have failed and that have not failed could be compared to try to identify specific causes of failure. This proposed analogue would be intermediate in time scale (50-100 years), since modern portland cement has been in existence for only about 100 years. An extensive data base on reinforced concrete should be available for 50-year-old concrete from World War II bunkers.

A possible test case that meets most of the criteria for evaluating this intermediate time scale is the Polish

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national waste disposal facility at Rózan. The Rózan facility was constructed between 1905 and 1910 as a fortification of the (then) Russian frontier. The fort consists of a number of "objects," which are currently being used for disposal of low-level and intermediate-level waste. Historical records and measurements are available that may allow quantification of degradation rates over an intermediate period. The concrete used at the site is not reinforced; interestingly, this may be an advantage for long-term performance of waste disposal facilities, since corrosion of the rebar tends to crack concrete, leading to increased saturated conductivities, and worse potential behavior for containing waste. That is, removing the rebar removes a long-term degradation mechanism at the expense of short-term strength.

Ancient cement structures would provide analogues over times closer to those needed for performance assessment; however, these structures are not recommended because (1) ancient concretes are not the same composition as modern concretes, (2) ancient concretes are not reinforced, and (3) it is important to have information about ancient concrete structures that have failed (for which records are probably not available), as well as those that are currently standing.

As discussed above, one potential drawback of this proposed test case is that concrete durability is strongly related to formation quality assurance and quality control issues, and therefore may not be easily used to study past structures. For example, two concretes could be of the same composition, but because of quality control during formation, one concrete may degrade much more rapidly than the other. Therefore, it may be difficult to attribute concrete structural failures to mechanistic processes. To address this concern, a sensitivity analysis using concretes formed under different levels of quality control could be conducted to try to quantify the effect of quality control on degradation. As discussed previously, existing information on these topics is related to properties that are of relatively little importance in performance assessments.

Research on barrier degradation has a high potential for providing information useful in performance assessments. However, failure of these barriers is primarily dependent on site-specific, design-specific, and construction quality features. Consequently, research on mechanical failure of engineered structures has a relatively low likelihood of providing generic information for use in performance assessment.

3.1.3 Leaching

Unstabilized waste is sufficiently heterogeneous and uncertain in its physicochemical properties that one cannot expect to develop a better understanding of its leach mechanisms. For stabilized waste, Kozak *et al.* [1990a] recommended the leach models described by Sullivan and Suen [1989]. These are a surface-wash model, a diffusion-limited model, a congruent-dissolution model, or any combination of these models.

There are geochemical models that have been developed to provide estimates of speciation and solubility in ground water, based on equilibrium chemistry. Besides their associated conceptual model uncertainties (e.g., assumptions about chemical reaction kinetics), these models require information about the chemical condition of the water in the disposal unit over time, which is likely to be uncertain. For example, many models use a simple parameter known as the Eh of the ground water to calculate the solubilities and speciation of radionuclides, yet there is no simple way to measure or to predict the magnitude of this quantity [IAEA, 1989]. Because of these uncertainties, geochemical models were not explicitly included in the methodology.

The most significant uncertainties associated with the leach models contained in the methodology result from the unknown geochemical nature of the ground water in the waste form, which is required to implement the leach models. It is clear that conditioning the waste to reduce the uncertainty in this chemistry will be useful. Since the waste itself is highly heterogeneous, the conditioning must be performed in one of two ways. Either the waste must be conditioned to remove its heterogeneity (as may occur after combustion or vitrification), or the chemical environment in the disposal unit must be dominated by an additive. For instance, designs that involve the use of large amounts of grout backfill may provide better confidence because the grout dominates the near-field chemistry. In this way, confidence in the chemical behavior of the system can be improved.

Validation studies for leach models and geochemical models of trash wastes are intractable, owing to the heterogeneous nature of the waste form. For this type of waste, the only defensible approach is conservatism. Therefore, validation efforts should be focused on stabilized waste forms. However, if performance assessment results indicate that certain radionuclides in the

trash waste are the most important, validation studies on trash waste may need to be revisited.

Key issues that should be addressed in validation of leaching models are (1) for what conditions and waste forms is the assumption of diffusional transport of a radionuclide through the waste form justified, and (2) can generic diffusion coefficients be used for some stabilized wastes? As discussed above, the leaching behavior of concrete-stabilized waste may be dominated by the chemical behavior of the concrete for a wide range of conditions. If this is true, it may be possible to reliably use *generic* leaching data to specify generic ranges of input parameters for specified types of stabilized waste. This would allow site-specific validation efforts to focus on other areas.

A potential validation test case to address these issues consists of comparing leach data from several different stabilized waste forms with available leach models. The applicability of the diffusional transport model can be established by using the different models. Such comparisons would either raise or lower generic confidence in the leach models for low-level waste performance assessment. A potential data set for use in this test case is a solidified waste lysimeter in operation at the Savannah River site [Vejmelka *et al.*, 1991]. The lysimeter consists of liquified waste solidified *in situ* in a concrete matrix. This lysimeter has been in operation for a number of years, and a significant amount of data has been collected. McConnell *et al.* [1991] and McIsaac *et al.* [1991] also have discussed leaching data that may be appropriate for a validation data set.

A better understanding of leaching phenomena has the potential for providing significant benefits in performance assessments. Furthermore, by standardizing designs, information of general applicability could be produced. This standardization would be derived primarily from near-field chemical effects.

3.1.4 Near-Field Chemistry

The chemistry in the disposal facility has the best potential for reliably reducing long-term releases from the facility. Chemical limitations on releases are not strongly affected by structural failure of the vault, nor even by significant changes in permeability. Indeed, the chemical behavior of the system can be expected to persist for very long times into the future. As a result, there is a strong incentive for treating the waste to limit its dissolution into water.

The CHEMVAL international study is attempting to address validation of geochemical models. The study consists of four stages: (1) verification of chemical equilibrium models, (2) attempted validation of speciation-solubility models by comparison with experimental field and laboratory data, (3) verification of coupled chemical transport models, and (4) attempted validation of coupled chemical transport models [Read and Broyd, 1991]. The third stage has been completed and the fourth stage is in progress. For the second stage, data from four sites were selected: the Mol site (organic-rich clay), the Gorleben site (actinide solubility experiments, using ground water from above the potential salt repository), the Maxey Flats site (a closed low-level waste facility) and the Oman site (highly alkaline spring waters, which may represent a cementitious environment).

The validation test case suggested for near-field transport models consists of three parts. First, as an initial step, the second stage of the CHEMVAL study should be assessed, especially the Oman data set. The Oman data set is based on a study by Bath [1987] which investigated alkaline ground water in Oman, near the Arabian Gulf, as a natural analogue for cement pore waters. Next, participation in the last stage of CHEMVAL should be considered for its relevance to the methodology. What is important is that only cementitious environments should be considered, since this area holds the prospect of generating some useful information for the low-level waste source term. Finally, information from the geochemical validation studies should be used to provide a generic basis for input parameters required in the near-field transport and leach models contained in the methodology for cementitious environments.

A first step in evaluating these effects is to establish the solubility limits and potential behavior of key radionuclides in cementitious environments. In addition, it is desirable to look for other possible additives that may influence the chemistry of the disposal facility in a positive way. In particular, the chemistry of iodine (^{129}I) and technetium (^{99}Tc) needs to be studied. These radionuclides are expected to predominate in anionic form, and special consideration for them may be merited. Treatment of these wastes may include pretreatment of the waste to control speciation of iodine and technetium, as well as modifications of waste forms to ensure that these forms continue to dominate under disposal conditions.

Designing the chemical environment of the disposal facility to reduce releases can have large benefits on facility performance. Furthermore, this area can be

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controlled through appropriate design, and long-term degradation of the facility will have only minor influences on the chemical environment. Consequently, research on chemical limitations to release can be expected to have generic applicability as well as generic importance.

3.1.5 Ground-Water Flow and Transport Within and Near a Disposal Facility

To determine the radionuclide source term, the flux of ground water into the disposal unit must be estimated. In the methodology, the unsaturated zone flow model based on Richards' equation is recommended for modeling ground-water flow within and around the disposal unit. Besides the uncertainties associated with the conceptual model, one of the most uncertain aspects of this type of ground-water flow modeling is in the input parameters. These parameters represent estimates of flow properties of the disposal unit, including any engineered cover or barriers, and are highly uncertain because of the heterogeneous nature of the disposal unit. For example, the configuration of the waste adds unknown spatial heterogeneities to the required flow input properties. The uncertainty in the flow properties of the waste, and the evolution of flow properties of concrete, are the two primary validation issues associated with near-field flow models. It is virtually impossible to address these validation issues owing to the inherent heterogeneities in low-level waste and facility characteristics, especially for long periods. Therefore, validation efforts should focus on the underlying conceptual model uncertainties associated with ground-water flow models.

Alternatives to the near-field transport models discussed above are coupled geochemical-transport models. The reason for this type of coupling is that the waste chemistry becomes important for simulating near-field transport processes (e.g., dissolution, sorption). The area where geochemical models seem most applicable is in disposal options with cementitious backfill, with the waste form grouted in place. In this case, the chemical behavior of the near field may be dominated by the cement, and the uncertainties associated with the *in situ* ground-water chemical conditions would be reduced. There are several issues that arise with this concept. For instance, if flow is dominated by cracks, its influence on the water chemistry is unclear. In general, near-field flow and transport analyses are subject to the same issues as the flow and transport modeling done for the hydrosphere.

Developments in this area are likely to have little effect on the ability to assess performance of a facility. Flow and

transport are primarily influenced by the manner in which a disposal facility degrades as a function of time, which provides boundary conditions for the flow analysis. Furthermore, flow and transport within a facility can be expected to be strongly influenced by site-specific features and phenomena. Consequently, research on near-field flow and transport is unlikely to yield information that has generic applicability to performance assessment.

3.1.6 Source Term Summary

Improvements to source-term analyses can be categorized as those that improve confidence in estimates of the mechanical containment of the waste, and those that improve confidence in estimates of the chemical containment of the waste. Mechanical containment consists of the areas of barrier degradation, and flow and transport of contaminants. Improvements in the understanding of these areas can be expected to have a significant impact on performance assessments, but such confidence is unlikely to be achieved in a generic sense. By contrast, an improved understanding of chemical limitations to release rates may lead to the ability to dominate the near-field chemistry in a favorable manner, regardless of site-specific conditions. Chemical limitations to release will persist for extended periods, and will not be strongly influenced by mechanical failure of a facility. Improved understanding of the near-field chemistry is the most promising area of research in low-level waste performance assessment.

3.2 The Hydrosphere

We begin the discussion of hydrosphere modeling by reiterating the points made earlier on general validation. First, true validation of models, and particularly of hydrosphere models, used for performance assessment is impossible. Second, hydrosphere models are invariably dominated by site-specific influences, which makes transfer of information from one site to another a difficult enterprise, fraught with uncertainty. Third, data sets used in hydrosphere modeling are unusually sparse, and unambiguous answers are rare. Based on these issues, it seems unlikely that improved generic confidence in hydrosphere models used in performance assessments will be developed soon, if ever. Consequently, we conclude *a priori* that hydrosphere validation exercises will tend to be less fruitful than perhaps will other performance assessment areas, and should therefore receive lower priority. Instead, hydrosphere modeling for performance assessments must be viewed as developing an adequate description of the site-specific conditions, with relatively

little assistance from generic studies. Nevertheless, it is worthwhile examining hydrosphere models, since they are of primary importance to the results of a performance assessment.

3.2.1 Infiltration

The flux of ground-water into the disposal facility is needed to estimate the source-term release. Estimating this flux consists of finding the amount of water that infiltrates into the soil, redistributes, and enters the disposal unit as a function of time. In the methodology, the infiltration rate of water into the soil is considered a boundary condition for a ground-water flow model, and this is used to simulate ground-water flow into and around the disposal unit.

Kozak *et al.* [1993] did not include a formal model for infiltration, since it is widely recognized that infiltration estimation is very site specific, and that specific models cannot be recommended in general [Gee and Hillel, 1988; Kozak *et al.*, 1989; Smyth *et al.*, 1990]. In addition, currently there is no consensus among practitioners concerning the applicability of infiltration models [Knutsson, 1988; Balek, 1988]. Nevertheless, a number of models do exist that can be used to estimate infiltration rates. These include water balance models [Perrier and Gibson, 1982; Schroeder *et al.*, 1982; Knisel, 1980; Fayer *et al.*, 1986] and tracer models [Eriksson and Khunakasem, 1969; Allison and Hughes, 1978; Edmunds *et al.*, 1988; Phillips *et al.*, 1988].

Water balance models estimate the different parts of the water budget (e.g., precipitation, surface run-off, evaporation, plant transpiration), where the residual is attributed to infiltration. Unfortunately, it is not possible to measure directly each one of these components (e.g., evaporation, plant transpiration). Therefore, mechanistic [Hillel and Van Bavel, 1976; Gupta *et al.*, 1978] and empirical models [Devries, 1984; Rosenberg *et al.*, 1983], as well as environmental tracer models [Allison, 1982; Knowlton *et al.*, 1989] are often invoked. Data requirements for such models include rainfall rates, temperatures, solar radiation, leaf area, and characteristics of the facility cover material [Kozak *et al.*, 1989]. Tracer models use information about tracer input and movement in the soil to estimate the amount of water infiltrated. The underlying assumption is that the movement of the tracer is a representative record of the infiltrating water. The tracer can either be introduced intentionally (e.g., dyes) or may be already present in the environment (e.g., nuclear bomb pulse tracers such as ^{36}Cl and tritium, and isotopes

such as ^{14}C and ^{18}O). Using tracer models to estimate infiltration rates appears to be valuable because the models are based on site-specific physical evidence (e.g., spatial tracer distributions in the soil). However, to obtain an infiltration rate, the physical evidence has to be interpreted, and several significant assumptions have to be invoked. Most tracer models are based on the assumption that flow is one-dimensional, that piston flow predominates, and that the tracer deposition and precipitation rates are constant or can be averaged [Stone, 1984]. Also, use of tracer analyses may be precluded for scoping performance assessment analyses since site-specific information about the spatial distribution of the tracer in the soil is required. Schulz *et al.* [1990] have demonstrated a field-scale test of several alternative cover designs; this kind of field-scale test may serve as a prototype for evaluating cover systems for individual sites.

Although these models for infiltration exist, there are large uncertainties associated with them. For water budget models, the most significant uncertainty centers around the inadequacies of direct measurements for the relevant components of the water budget, especially for evaporation and plant transpiration. Therefore, the uncertainty that is associated with each component model (input parameter and conceptual model uncertainty) is propagated through to the final estimate of infiltration. In general, uncertainties arise because of climatic variations, and variability in soil and vegetation [Smyth *et al.*, 1990]. Freshley *et al.* [1985] indicate that spatial and temporal variations in precipitation have the greatest effect on infiltration rates, and based on lysimeter data, Jones *et al.* [1988] also observed that infiltration was highly dependent on climate variations. The effect of soil and vegetative variability was shown by Gee *et al.* [1989], where different soil lysimeter covers (fine versus coarse) and different vegetation resulted in a dramatic effect on infiltration, with climatic conditions being constant. The uncertainty associated with tracer models includes uncertainty in the initial source term (e.g., history of bomb-pulse tracer release and deposition), and uncertainty associated with the conceptualization of tracer flow in the geologic medium.

Besides the uncertainties discussed above, there is also uncertainty associated with estimating infiltration rates for the relatively long assessment time periods. In other words, to estimate an infiltration rate, an assumption about the future state of the system, which is uncertain, has to be made. There are many processes that can occur over time at the land surface (e.g., climate change, vegetation change, erosion) that can significantly affect estimates of

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infiltration. One of the main issues for performance assessment concerning infiltration is the question of how to use short-term, uncertain temporal and spatial information about infiltration (whether from a model or measured) to model the system for the relatively long assessment periods. Assumptions about long-term infiltration translate into specific assumptions in modeling ground-water flow for performance assessments (e.g. steady-state flow, where infiltration is approximated as a constant flux or constant head boundary condition).

It is clear that estimating infiltration is a site-specific exercise. Developing confidence in particular approaches at specific test sites [e.g., Schulz *et al.*, 1990] does not necessarily build confidence in the relative effectiveness of those approaches at other test sites. We therefore conclude that validation exercises on infiltration will be of relatively limited usefulness in developing generic confidence in performance assessments.

3.2.2 Ground-Water Flow and Transport

The dominant model that forms the basis for virtually all ground-water flow and transport analyses is Darcy's law, including Richards' extension to unsaturated media. These models represent an assumption of linearity between a pressure driving force and specific discharge of fluid. It is well known that Darcy's law fails at both low and high flow rates (for differing reasons) and when other driving forces for flow become important, such as osmotic phenomena. However, these conditions are comparatively rare in practice, and will not be considered further here. In the intermediate range of ground-water flow rates in porous media, Darcy's law is generally accepted without significant question by practitioners of performance assessment.

Several more important issues are subject to intense research efforts around the world. Of particular importance for performance assessments of low-level waste disposal facilities are (1) scale and heterogeneity effects, (2) constitutive relationships for unsaturated flow, (3) determination of boundary conditions, (4) dispersion, (5) flow in fractured media, and (6) the relationship between ground-water concentrations and well-head concentrations. These areas are intertwined at many levels, and are frequently indistinguishable. The bases for each of these research areas are the extreme paucity of data with which ground-water analysts must deal, and the extreme heterogeneity of subsurface features at all scales.

3.2.2.1 Scale and Heterogeneity

Natural porous media are heterogeneous at all scales by definition, since they consist of voids and solids, and because the arrangement of the voids and solids is generally nonuniform. If one knew the distribution of voids and solids, so that boundary conditions could be established, a continuum for each phase could be assumed on the pore scale. However, this information is not available; therefore, an initial objective of modeling flow and transport through porous media becomes the establishment of a scale at which a continuum can be assumed, and information about pore-scale heterogeneity is no longer required. In this approach, continuum equations are developed for the porous medium, which implicitly contains the continuum effects of each phase.

Understanding the scale at which continuum effects can be assumed traditionally been done by using the representative elementary volume (REV) concept [Bear, 1972]. The REV scale can be described as a scale where, whenever a measurement is taken, both voids and solids exist [Bear and Verruijt, 1987]. If the scale is smaller than the REV, measurements will fluctuate; sometimes voids will be observed and sometimes solids will be observed. If the scale is larger than the appropriate REV, measurement fluctuations will again be seen because of the influence of boundaries or different facies, or because the scale is so large that it is not in the domain of interest. The basic underlying assumption is that the relevant variable does not depend on the magnitude of the REV as long as the REV is sufficiently large; therefore, a quantitative definition of the REV size is not required [Dagan, 1986]. This REV averaging of pore-scale heterogeneities allows the application of continuum mechanics. The continuum mechanics equations for momentum, heat, and mass transport are the basis of all ground-water flow and transport models. Although information about the pore-scale heterogeneity is not needed, instead coefficients related to the new averaged scale are required. The scale at which ground-water flow and transport models are used for a performance assessment is relatively large. Therefore, although the REV concept presents a logical framework to go from the pore scale to the laboratory scale, there is some question whether laboratory-scale results are applicable to the field scale. Related to this scale issue is the pragmatic need to establish the usefulness of laboratory measurements in modeling ground-water flow and transport models. Laboratory methods provide a convenient means for

studying ground-water flow and transport because of their inherent economic and logistic advantages [Taylor *et al.*, 1987]. Therefore, it is necessary to relate laboratory measurements to field observations. This is especially relevant for low-level waste disposal, where economic considerations may preclude extensive field testing at each proposed site. Nevertheless, there is a need to establish when the regulator should require extensive field testing.

Traditionally, the required model coefficients are found by laboratory measurements on samples of the large-scale geologic porous medium, and these coefficients are then applied to field-scale modeling. This approach is based on the assumption that the large-scale porous medium is uniform with respect to these variables. However, as noted by Dagan [1986], this is not supported by field observations, which indicate that these coefficients vary over space. These variations can be addressed by appropriate use of uncertainty analysis, which provides a conceptual framework for dealing with unknown spatial heterogeneities. The underlying question of how to use data measured at different scales remains.

Based on the above discussion, it is apparent that there are uncertainties in the underlying theoretical basis for ground-water flow and transport models. These uncertainties, which correspond to validation issues, result because model variables cannot be directly measured, and because they are based on an averaged scale that cannot be specifically defined. Therefore, measurements of these quantities at the laboratory scale are questionable when applied to the field scale. Consequently, field-scale parameters have to be interpreted by invoking or calibrating a model (e.g., pumping tests).

The main validation issue reduces to relating the experimental measurement scale to the "averaged" scale needed to apply the model. Traditionally, model input is either based on the experimental results (calibration), or on and interpretation of experimental results with another model. For example, in a pumping test, an estimate of the hydraulic conductivity is usually based on the Theis model, and for permeameters, hydraulic conductivity estimates are based on Darcy's law. When the input is dependent on experimental results, the only way to build confidence in ground-water flow and transport models is by a two step process: (1) calibration, and (2) using the calibrated input to attempt to predict results for the same experiment conducted under different conditions.

3.2.2.2 Constitutive Relationships for Unsaturated Flow

Validation issues related to the underlying theory of ground-water flow and transport models also apply to unsaturated ground-water flow models. These issues include the determination of effective "average" flow and transport material properties to use when modeling flow through unsaturated, heterogeneous geologic media. This issue is probably the most significant since it is the basis for the models. More specific validation issues for vadose zone ground-water flow and transport models include (1) the validity of the models used to estimate the relationships between the moisture content, pressure head, and unsaturated hydraulic conductivity, and (2) the dependence of dispersion and retardation on moisture content. The uncertainty associated with unsaturated hydraulic conductivity estimates is probably much more significant than the dependence of dispersion and retardation on moisture content.

To address the first validation issue, a potential validation test case would consist of taking existing moisture content, pressure head, and unsaturated hydraulic conductivity data and comparing these data with the available models (e.g., van Genuchten, Mualem, Brooks-Corey). The novelty in this test case would be the application of a formal validation strategy, including parameter uncertainty analysis and a quantitative acceptance criteria. However, it should be noted that it is very difficult, if not impossible, to estimate unsaturated hydraulic conductivity at extremely low moisture content (i.e., high suction heads) although tracer or centrifuge techniques have been suggested.

3.2.2.3 Boundary Conditions

As with most mathematical models of physical processes, the boundary conditions imposed on performance assessment analyses produce dominating effects on the outcome of the calculations. The boundary conditions of importance for ground-water flow and transport analyses have uncertainties in them that result from one of several reasons. First, the subsurface contains spatial heterogeneities that make the spatial location of any imposed condition (such as a no-flow boundary) uncertain. This problem is made particularly acute in ground-water analyses because of the paucity of data available for such systems. Second, performance assessments are invariably

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conducted using a steady-state flow model. Extracting steady-state boundary conditions for intrinsically transient phenomena clearly introduces an additional level of uncertainty. One example of this kind of uncertainty is the difficulty in estimating recharge from transient rainfall and evapotranspiration information. Third, there are frequently no natural boundary conditions that can be applied on any reasonable scale for performance assessment. An example of this is the analysis of low Peclet number problems, in which diffusion and dispersion are of comparable importance to convection. In this case, it is very difficult to assign a boundary condition on concentration anywhere in a reasonably sized domain, because the boundary conditions tend to be influenced by the phenomena between the boundaries. An approach for treating this problem, in principle, is to apply continuity conditions between solution domains on either side of a boundary, rather than boundary conditions, which are imposed *a priori*. Fourth, uncertainties can be introduced by the manner in which the problem is subdivided for analysis. Performance assessments are usually subdivided into modules. Between each of these modules, implicit boundary conditions are usually applied. For instance, if the analysis is subdivided into vadose-zone and saturated-zone analyses, they must be linked so that releases from one zone form releases into the next. Physically, the only conditions that apply at the interface between vadose and saturated zones are continuity of mass, energy, and momentum. However, as a modeling simplification, other conditions (e.g., zero concentration, zero gradient of concentration) are commonly applied to allow separation of the two zones into separate calculations. As a consequence, the potential exists for nonphysical discontinuities at module interfaces.

The uncertainties associated with these effects are too diverse and widespread throughout performance assessment modeling to admit any general solution. Consequently, they must be resolved on a site-specific and analysis-specific basis, through intercomparison of models and corroboration by data. The effect of misapplying boundary conditions in performance assessments has not been carefully studied, and deserves some attention.

3.2.2.4 Convection, Dispersion, and Retardation

The most popular transport model is the convective-dispersion mass balance equation. There are several implicit assumptions associated with this model. They include (1) the effects of concentration, temperature, pressure, and multiple components (cross-term effects), which are neglected for molecular diffusion, (2) the

hydrodynamic mechanical dispersion process is assumed to be Fickian, and (3) all the chemical processes that may affect transport are represented by a retardation factor, which is usually based on a linear distribution coefficient.

The first assumption is not usually significant, owing to the trace amounts of contaminant usually encountered in performance assessment, and because molecular diffusion is usually not the dominant transport process in ground-water systems. However, these assumptions may become more significant for gas-phase transport, and for diffusion-dominated transport in clays.

The second assumption, assuming that dispersion is a Fickian process, is one that is usually accepted in practice. However, similar to Darcy's law, there exists the need to compile the supporting evidence for this relation. Gelhar [1986] notes that application of the stochastic models does not assume that the large-scale dispersion transport process is Fickian. Instead, it is shown that this process can be simulated knowing the spatial variability of the hydraulic conductivity parameter. Regardless, it is clear that the dispersion process is significantly affected by the underlying assumptions concerning scale. The reason for this is that dispersion is not a physical phenomenon, but rather is an informational one. Dispersion is a model representation of an averaging process over unknown variations in velocity. Consequently, it is a model-based process that is not useful for prediction.

The last assumption related to the convective-dispersion model is significant for performance assessment, since large distribution coefficients are often measured in the laboratory and used in performance assessment models, thereby leading to estimates of significant retardation. Retardation may significantly increase the arrival time of the contaminant at the point of compliance, which can allow greater time for decay. Consequently, accounting for retardation is not usually conservative. However, in some unusual cases, such as two vaults failing at different times, retardation of one component may lead to an overlap of arrival times that would otherwise be separated.

3.2.2.5 Fractured Media

Flow and transport in fractured systems are important for low-level waste performance assessment in one of two ways. First, current disposal designs call for the use of concrete vaults to assist in confining the waste. Over extended periods of time, the concrete is expected to fail hydraulically by progressive development of cracks. Consequently, simulation of flow in such unsaturated

fractured systems is important for evaluations of releases from the facility. Second, the potential exists for new facilities to be sited in a geological setting characterized by fractured rock. This situation is believed to be of lesser importance than the concrete fracturing issue, since most States' and Compacts' siting processes appear to discourage siting in fractured geological media. The reason for this is the increased uncertainty in the performance assessment modeling of fractured media.

Extensive research programs already exist for studying flow and transport in fractured media. Consequently, additional research in this area is not expected to have a large impact on performance assessments. For low-level waste performance assessments, the issues related to fracture formation and propagation in concrete can only be studied over the time frame of the performance assessment. It is possible that studies of old and ancient concrete structures may shed some light on this area. However, this area of research is not expected to produce results significant for current performance assessments, because of the crude representations of flow through concrete that are currently accepted.

3.2.2.6 Relationship of Ground-Water and Wellhead Concentrations

Another validation issue for saturated-zone flow and transport models in the methodology concerns the relationship between ground-water concentrations and well-head concentrations. A drinking-water well in a performance assessment calculation is rarely, if ever, treated as a pumping well in an aquifer simulation. Instead, it is more typical to model the wellhead concentration in one of several simplified ways. Most commonly, it is assumed that the maximum concentration in the aquifer is what is consumed from the well. In this approach, the well is viewed as a monitoring well, which does not significantly affect the general flow field. An alternative approach is to calculate a discharge rate to the well, and to dilute that discharge rate by either a well pumping rate or some aquifer flow rate. Using a well pumping rate is equivalent to an assumption that the well capture zone is larger than the dimensions of the plume. Using an aquifer flow rate invokes an assumption about the behavior of transverse dispersion in the aquifer.

Using the maximum concentration in the aquifer is generally thought to be a conservative assumption, but this must be tested. A potential method for evaluating the conservatism of this approach would be to compare wellhead concentrations from alternative approaches under a variety of conditions. However, the generality of such

an approach would always be suspect. Consequently, it appears to be more efficient to evaluate these effects on a site-specific basis.

3.2.3 Surface-Water Transport Models

Jirka *et al.* [1983] have discussed the details of surface-water transport models that may be appropriate for performance assessment analyses. Surface-water pathways associated with low-level waste disposal facilities tend to be of relatively minor importance relative to the ground-water well pathway. As we have discussed elsewhere [Kozak *et al.*, 1993], the consequence of this limited importance is that surface-water transport analyses can often use models that exclude many of the most complicated phenomena. Such screening models are often sufficient for analyzing surface water doses. They are adequate for performance assessments to the extent that they can be demonstrated to be conservative.

The most significant validation issues for surface-water transport are mixing of contaminants in large surface water bodies, and the interaction of contaminants with the sediments. If significant sorption occurs, sediment settling, scouring and transport may become important. However, the relative importance of contamination in sediments must be determined from an assessment of the overall pathway to humans. Exposures to sediments are likely to be important only in unusual circumstances. Examples of such circumstances might be if bottom-feeding fish are an important constituent in the local diet, or if sediments are commonly exposed to the air.

Although there are many measurements that have been made in the Columbia, Clinch and Savannah rivers, there are very few data sets extensive enough to be used for validation studies [NCRP, 1984]. Onishi *et al.* [1981] have accumulated and tabulated the available data sets and their work indicates that the data are sparse. The problem seems to be that there are few surface-water systems where sufficient concentrations of radionuclides have been or are being released [NCRP, 1984]. However, there are two possible exceptions: (1) release of fission products and transuranic elements from the Windscale plant into the Irish Sea [Hetherington *et al.*, 1975], and (2) residual activity measured in the Great Lakes resulting from atmospheric nuclear weapons tests.

3.3 The Atmosphere

In low-level waste performance assessments, the atmospheric pathway generally produces very small doses.

Validation

As a result, it is frequently possible to use very conservative assumptions for demonstrating compliance. Chu *et al.* [1990] have described a typical conservative modeling approach, in which variability of wind speed, direction, and stability are all neglected. It appears that the use of bounding assumptions such as these will be the rule rather than the exception for low-level waste performance assessments. The form of the model (a Gaussian plume) does not appear to be seriously questioned by performance assessment practitioners. It is therefore clear that validation issues in air-transport models will be of very minor importance for low-level waste performance assessment. Modifications to initially conservative analyses can generally be easily justified using site-specific information about atmospheric conditions and duration of exposure. The key issue related to the air-transport pathway is the rate of release of contaminants into the gas phase. Issues related to gaseous releases were addressed in Section 3.1.

3.4 The Biosphere

3.4.1 Environmental Pathways

For determining radionuclide intake rates for an individual from concentrations in the environment, Kozak *et al.* [1990a] suggest the pathway models found in NRC Regulatory Guide 1.109 [NRC, 1977a]. Alternative modeling approaches are similar to the Regulatory Guide approaches, with subtle differences in models and default parameters [Napier *et al.*, 1988; Kennedy and Strenge, 1992; Merrell *et al.*, 1986]. In general, all of these approaches consist of chains of linear multiplication factors that translate concentrations in various exposure media into intake rates in humans.

The most significant validation issue for food-chain models centers on bioaccumulation of radionuclides, especially for ^{14}C compounds. The NCRP [1984] states that few efforts have been made to validate the bioaccumulation values listed in regulatory guidance, and that validation studies are needed because those in the regulatory literature are believed to be overly conservative. Other validation issues include the lack of isotope-specific transfer coefficients for specific foods. However, conservative assumptions should overestimate concentrations in terrestrial foods and bioaccumulation factors in aquatic food chain transport models. In addition, food consumption parameters are based on 1965 data; given the change in U.S. dietary habits since then, these values are quite suspect [NCRP, 1984]. Since these

habits will continue to evolve in unknown ways in the future, regulatory authorities must make policy decisions to define a set of conditions that can be used to make regulatory decisions.

One study concerning food-chain transport was the international BIOMOVs study [BIOMOVs, 1990]. The initial case studies included releases of contaminants into rivers, air, ground water, and lakes, with subsequent uptake into the ecosystem. In addition, contamination of the terrestrial food chain generated from the Chernobyl accident was included in a test case. These test cases have been completed, and BIOMOVs 2 is under way. Several areas were identified as possible candidates for case studies for this second phase [BIOMOVs, 1990]. These areas are (1) multihazard risk analyses, (2) temporal evolution of the biosphere, and (3) additional work on impacts of Chernobyl on surface-water and terrestrial ecosystems. Specific details of the test cases are not available to us at present.

These types of databases would be very useful for validation test cases for common pathway analysis models. At present, pathway analysis codes like GENII have generally not been subjected to validation. GENII was developed for the Hanford site using site-specific parameters, but little process model validation has been done on the code. Recent comparisons between GENII and alternatives like PATHRAE [Merrell *et al.*, 1986] have shown differences that may be linked to site-specific environmental parameters in either or both of the codes. These problems can in all likelihood be resolved by careful inspection of the underlying model assumptions. However, there are apparently also differences in some of the process models [Baird *et al.*, 1990]. These differences can be resolved only by experimental data.

A useful approach to developing generic confidence in environmental pathway assessments would be to evaluate the uncertainty in output concentrations for ranges in input data. This could be accomplished by a program that critically reviews the input data requirements for the exposure analysis models, with a view toward establishing the level of current scientific uncertainty. These uncertainties can then be propagated through the models using standard approaches for propagating parameter uncertainties. Since the models for this portion of the performance assessment are linear, it is likely that the sensitivities can be determined analytically, without recourse to Monte Carlo methods. The result of such an exercise would be an identification of the parameters and models whose uncertainties result in the most important

uncertainties in model output. These uncertainties would then define an appropriate direction for further experimental work.

3.4.2 Dosimetry

Once the intake of radionuclides for a person has been established based on food-chain models (see Section 3.4.1), dosimetry models are needed to estimate the effect of this intake on the human body. In the methodology, internationally accepted dosimetry models [ICRP 26, 1987; ICRP 60, 1990] are used which are based on dose conversion factors [ICRP 30, 1982-1988].

The primary validation issue surrounding dosimetry modeling is the following: Are the current dose models "good enough" to be used to make acceptable regulatory decisions? From a regulatory perspective, one only needs to explicitly define the performance measures in 10 CFR Part 61.41 as referring to the Standard Man, and dictating the use of the standard dose conversion factors.

These questions are directly related to regulatory policy rather than technical issues, and so are not discussed further here.

For a potential validation test case, we recommend that the uncertainties in the ICRP dosimetry methodology be identified and propagated, to quantify the likely range of possible values of dose conversion factors. Such studies may include determining variability about the Standard Man for the standard assumptions used in defining the Standard Man, as well as determining gender, race, and age variabilities. This information should be developed for the sake of generality, but it is not clear whether it would (or should) have an impact on low-level waste performance assessments. From a performance assessment perspective, dose conversion factors are used only to translate concentrations into a number that is presumed to be related to risk. The dose value thus calculated does not, and need not have any close relationship to a real dose to a real person, provided that it is a conservative estimate.

4.0 Summary and Ranking of Validation Requirements

Performance assessment has been shown to be a general approach for supporting an assessment of compliance of a disposal facility with pertinent regulatory standards. Performance assessment cannot be regarded as a scientific demonstration of site safety, since the scientific method is of limited usefulness in low-level waste performance assessments.

Traditional validation exercises have been shown to be applicable to developing generic scientific confidence in types of behavior that are expected to occur at waste disposal facilities. They have very limited usefulness for developing confidence in a particular performance assessment. Indeed, it has been argued that validation studies should only be used in a performance assessment to reduce the initial scope of phenomena that must be

considered, and so make the process more efficient and less costly.

Performance assessment models have been subdivided into several areas. The potential for validation studies to affect performance assessments in a positive way has been assessed, with the results shown in Table 4.1. The most important areas in which focus is needed are as follows: Research into the disposal facility chemistry may be used to develop better confidence in assessments of chemical limitations to release and transport over a long time. Research into the biosphere models will provide a better assessment of the uptake and importance of radionuclides (particularly ^{14}C) in various biological species, including humans. Such information will permit better confidence in the results of bioaccumulation analyses.

Table 4.1 Relative ranking of categories of performance assessment models

	Disposal facility flow	Disposal facility chemistry	Hydrosphere	Atmosphere	Biosphere
Amount of impact	High	High	High	Low	High
Potential for producing generic improvement	Low	High	Low	Low	High

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