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Waste Package Reliability

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ABSTRACT

Probabilistic Reliability Analysis is identified as the preferred method to identify, organize, and convey the necessary information to meet the NRC standard on reasonable assurance of waste package performance according to regulatory requirements. The document addresses both the qualitative and quantitative aspects of the analysis, and suggests reliability analysis requirements by a prospective license applicant as well as review procedures by the regulatory agency. In particular, a method for the quantitative evaluation of a waste package reliability is demonstrated through a simplified analysis. The method is based on the repetitive usage of a performance model for values of the model parameters that span their range of uncertainty. Techniques for selecting values of the input parameters, viewed as random variables, and for generating empirical correlations among experimental data are also described. Aspects which would need to be covered in a more comprehensive document are indicated.

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EXECUTIVE SUMMARY

The Code of Federal Regulations in its Part 10 CFR 60 §60.113 (June 1983) requires that the applicant for a license to operate a nuclear waste repository demonstrate compliance of the proposed design with performance criteria of individual barriers after permanent closure concerning containment and controlled release of the radioactive waste.

Although these performance criteria are quantitative, because of the uncertainties involved in predicting performance for thousands of years, NRC will not require absolute proof that these criteria are satisfied. What is required is "reasonable assurance, making allowance for the time period and hazard involved, that the outcome will be in conformance with those objectives and criteria."[1] "Reasonable assurance" is a term of law rather than a term of science. However, while it is recognized that reasonable assurance cannot be characterized with the degree of certainty implied by statistical definitions, 10 CFR 60 does expect the applicant to present calculated probabilities of meeting the Commission's criteria. The quality of the supporting evidence will be then a determining factor in the licensing decisions which the Commission will be called upon to make.

This document proposes the general method of probabilistic reliability analysis as an acceptable framework to identify, organize and convey the necessary information to satisfy the standard of reasonable assurance of waste package performance according to the regulatory requirements during the containment and controlled release periods. Based on available guidelines from References [2] and [3], suggested requirements for reliability analysis have been proposed. In particular, the analysis should be subdivided into two complementary parts encompassing qualitative and quantitative elements respectively. Qualitative analysis provides an identification of the various failure modes that contribute to waste package unreliability; quantitative analysis utilizes available experience on waste package components and their interactions and provides a numerical value of the probability that the waste package will perform its intended mission.

The proposed, main operational tool of qualitative reliability analysis is the failure modes and effects analysis - FMEA. This should be an integral part of the early design evaluation and should be periodically updated to reflect changes in design or application. These FMEA's often uncover hidden faults and weaknesses which can be corrected early in the design process or suggest relevant areas where further experimentation is required.

The core of quantitative reliability analysis is the uncertainty analysis which deals with the quantification of uncertainties in parameters, models, and in the degree of completeness of the implemented approach as well as the propagation of the uncertainties in the analysis. While it is recognized that uncertainty analysis lacks mathematical rigor, it is nevertheless recognized that it offers valuable tools in decision making, as testified by its use in the licensing of commercial nuclear power plants.

In particular this document, through an example of a simplified waste package-reliability analysis, shows that at least one technique exists - namely, Monte Carlo simulation - for uncertainty propagation and for calculating the probabilty of a waste package to perform its intended mission.

1. INTRODUCTION

1.1 Background Information

1.1.1 Waste Package Performance Criteria

The Code of Federal Regulations in its Part 10 CFR 60 §60.113 (June 1983) requires that the applicant for a license to operate a nuclear waste repository demonstrate compliance of the proposed design with the following performance criteria of individual barriers after permanent closure:

1. Containment of HLW within the waste packages should be substantially complete for a period to be determined by the Nuclear Regulatory Commission. Such a period shall be no less than 300 years and no more than 1,000 years.

2. The release rate of any radionuclide from the engineered barrier system following the containment period should not exceed one part in 100,000 per year of the inventory of that radionuclide calculated to be present at 1,000 years. Exception to this rule is allowed for radionuclides whose release rate is less than 0.1% of the calculated total release rate limit, which is taken to be 1 part in 100,000 per year of the (total) inventory of radioactive waste that remains after 1,000 years of radioactive decay.

3. Pre-waste-emplacement groundwater travel time along the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment should be at least 1,000 years or such other travel time as may be approved or specified by the Nuclear Regulatory Commission.

Although the controlled release requirement is on the engineered barrier system (the waste package and the underground facility), it is expected that the applicant will rely primarily on the waste package portion of the system. Thus, waste package performance is the direct concern of 2 out of 3 NRC individual-barrier performance criteria.

1.1.2 Proof of Compliance with the Regulatory Criteria

While the above performance criteria are mandatory, the NRC will not require absolute proof that these criteria are satisfied. What is required rather is "reasonable assurance, making allowance for the time period and hazard involved, that the outcome will be in conformance with those objectives and criteria."[1] The Commission has applied equivalent language in other contexts before, e.g., the licensing of nuclear reactors.

The Reasonable Assurance Standard is prompted by the qualitative finding of "adequate protection" to the health and safety of the public that the Commission has to issue for licensed activities under the provisions of the Atomic Energy Act. This standard has been approved by the Supreme Court and it allows the Commission the necessary flexibility to make judgemental distinctions with respect to quantitative data which may have a large uncertainty (in a mathematical sense). Thus "reasonable assurance" is a term of law rather than a term of science. However, while it recognizes that reasonable assurance cannot be characterized with the degree of certainty implied by statistical definitions, the rule does expect the applicant to present calculated probabilities of meeting the Commission's criteria. The quality of the supporting evidence will be then a determining factor in the licensing decisions which the Commission will be called upon to make.

1.2 Probabilistic Reliability Analysis

In recent years Probabilistic Risk Assessment (PRA) has been the preferred method to identify, organize, and convey the necessary information to meet the equivalent NRC standard on reasonable assurance for nuclear power plants. Generic guidance on how to perform a PRA is provided in the NRC report NUREG/CR-2300 "PRA Procedure Guide."[2] In particular, since the NRC criteria on waste package performance do not address risk to humans, Probabilistic Reliability Analysis, which is an integral part of any PRA, is the proposed technique to satisfy the NRC standard on reasonable assurance for waste packages.

Probabilistic Reliability Analysis addresses the probability that a system or a system component will perform its intended mission under stated conditions. As explained later, this analysis does not provide definitive answers or rigorous solutions in a statistical sense. However, it does afford a disciplined approach towards addressing the inherent reliability of a system and provides valuable insight to the system weaknesses and strong points, which works to the advantage of both the applicant and the regulator.

Probabilistic Reliability Analysis is usually presented in two parts encompassing qualitative and quantitative elements, respectively. Qualitative analysis provides an identification of the various failure modes that contribute to a system unreliability; quantitative analysis utilizes available experience on the system components and their interactions, and provides a numerical value of the probability that the system will perform as originally intended.

Until a waste package reliability guide is proposed, guidelines on waste package qualitative and quantitative reliability analysis should be extracted from the pertinent literature on nuclear power plants. To that effect, References [2] and [3] should prove helpful.

1.2.1 Qualitative Reliability Analysis

Depending on the stages of a system design, a qualitative reliability analysis is performed with one or more of the following objectives:

(1) to identify weak points or imbalances in the design
(2) to aid in the systematic assessment of overall system safety
(3) to document and assess the relative importance of all identified failures
(4) to develop discipline and objectivity on the part of a designer of safety-related systems
(5) to provide a systematic compilation of data as a preliminary step to facilitate quantatitive analysis.

To that effect, three operational steps have been proposed:[3]

(1) identify significant failures and their consequences (generally called Failure Mode and Effect Analysis - FMEA),
(2) display the above information in a table, chart, fault tree or other format, and
(3) evaluate overall system reliability relative to the information above, including data uncertainties, and resolve identified problems.

These qualitative procedures often uncover hidden faults and weaknesses which can be corrected early on in the design process or suggest relevant areas where further experimentation is needed.[4] In particular, as it is suggested in Reference [3], the FMEA should be an integral part of the early design evaluation and should be periodically updated to reflect changes in design or application.

Extended Qualitative Reliability Analysis

Other procedures devised to complement an FMEA as possible design and analysis tools are the common-mode-failure analysis (CMFA) [3,4] and cascade-failure analysis.[3] In particular, a CMFA is designed to identify mechanisms and modes of failures of components normally considered to be redundant, while the cascade-failure analysis is intended to identify failures which can lead to "chain-type" events.

1.2.2 Quantitative Reliability Analysis

Quantitative reliability analysis is performed with the objective to obtain a numerical value of the probability that the system will perform as originally intended.

The core of quantitative analysis is the uncertainty analysis, which addresses the quantification of uncertainties in parameters, models, and degree of completeness of the implemented approach, as well as the propagation of the uncertainties in the analysis. Sensitivity analysis, which entails the

determination of how rapidly the output of an analysis changes with respect to variations in the input, is a useful adjunct to uncertainty analysis. Both analyses are discussed next.

Uncertainty Analysis

Three types of uncertainties can arise in performance assessment: uncertainties in parameter values, uncertainties in modeling, and uncertainties in the degree of completeness. Parameter uncertainties arise from the need to estimate parameter values from data which are usually incomplete and from which the analyst must make inferences. Model uncertainties stem from the inadequacy of the various models to represent reality and from the approach used to estimate probabilities and consequences. Completeness uncertainties are related to the ability of the analyst to evaluate exhaustively all contributions to unreliability of a system. They refer to the problem of assessing what has been omitted, and might be regarded as a type of modeling uncertainty, although a special one.

While the above considerations are general in nature, one of the major difficulties in applying statistical methods to uncertainty analysis is that there exist two approaches to statistics: the classical or frequentist approach and the Bayesian or subjectivist approach. These approaches would usually obtain numerically similar results for best estimates and uncertainty bounds given sufficient data and the same modeling assumptions. The frequentist however will find it impossible to make quantitative estimates that cannot be based on data but must be based on experience in related areas, engineering analysis, and/or engineering judgement. The subjectivist will in general find it easier to express uncertainties quantitatively in those circumstances, but since his assignment of probability is subjective he may have difficulty in convincing others of his assignments. Both the subjectivist and frequentist approaches are addressed in Reference [2]. The noted NRC-Reactor Safety Study [5] WASH-1400 was based on the Bayesian approach.

A useful reference on uncertainty analysis and on techniques to be used is the NUREG report "PRA Procedure Guide".[2] It is noted in there, that uncertainty analysis still lacks "a generally accepted, rigorous mathematical

basis. Thus, the theory of statistics, with which uncertainty analysis is often identified, only provides tools and guidelines for dealing with those quantities, but it is in general too restrictive to satisfy the needs of the uncertainty analyst." Nevertheless this lack of rigor is not as serious as it may seem, as much of the value received from performing a reliability analysis is derived from the act of doing the analysis.[4] This is especially true for the qualitative elements of reliability analysis. Furthermore, as quantitative methods are used to analyze the results of the qualitative procedures, they allow the most important areas to be highlighted, resulting in the formulation of the most effective action to improve design reliability. As a result, a high inherent reliability can be developed in system and component designs. Thus, even if quantitative methods cannot demonstrate absolute compliance with a given performance criterion, they are effective tools in decision making.

Sensitivity Analysis

Sensitivity analysis determines the impact that changes in the input may have on the output of a performance assessment. If a parameter or a model is important to the final outcome of a performance analysis, and it is determined that the parameter or model uncertainty is large, this alerts the designer to design around this difficulty or to conduct further tests to decrease the uncertainty.

Sensitivity analysis techniques are touched upon in Reference [2].

1.3 Proposed Approach to Waste Package Reliability Analysis

Major components of the waste package system are the primary waste form, the waste form container, and packing materials. Ideally, it would be desirable to predict the performance of such a complex system during the operational life of a repository through the aid of comprehensive, fully deterministic models which span all possible failure modes in the presence of the evolving near-field environment. The usage of such models should be warranted by the availability of an adequate data base which provide values of the relevant model parameters with a sufficient degree of accuracy. In practice however, only a few simplified models have been presented in the literature, and

the relevant data have a great degree of uncertainty. Therefore it seems more appropriate, at present, to resort to a scheme to predict failure probabilities based on the application of simple phenomenological models. In this scheme, one identifies a radionuclide release scenario, formulates and justifies the relevant models, determines ranges and distributions of the associated parameters viewed as random variables, samples among these according to a probabilistic technique, and determines the predicted failure times. Reliability is then calculated.

In broader terms, the proposed approach for evaluating the reliability of a high-level waste package consists of the following steps:

1. Identifying the types of known failures that, on the basis of engineering judgement, are physically possible for the waste package for a given repository system in the sense of not violating physical laws. This is done on the basis of an exhaustive review of the relevant literature and exploratory experimentation under the guidance of general principles and existing knowledge of failure types in other systems which have points of similarity with the system under consideration. The process of identification is complete when independent reviews fail to reveal new possible failure types.

2. Evaluation and preliminary dismissal of those processes which are physically possible under some conditions but physically impossible under the repository conditions. For example, a type of corrosion of metallic components may be possible in a salt environment but not possible in a basalt environment. This process is complete when all failure types previously identified are either dismissed or explicitly retained for further analysis. The reasons for dismissal in each case are documented with defensible arguments, and in sufficient detail so as to facilitate subsequent reviews and possible reevaluations.

3. For each of the failure types retained for further analysis, a model is constructed. The model describes the conditions which may lead to the failure, predicts when the failure may occur, and the immediate results of the failure. The nature of the failures, the state of

knowledge, and the role of the individual failure in the overall failure of the repository dictates the level of detail required and the model uncertainty which is tolerable. This process is complete when for each of the failure modes there is a model and the model is documented, not only as to nominal values but as to statistical uncertainty and distribution forms of the predictions.

4. Properties describing the environmental conditions of the repository and parameters which are relevant to the selected models are analyzed and their values are measured or calculated. This process is complete when the links between observable and measurable properties and parameters of the repository system are identified, their values and uncertainties obtained, their probability distributions ascertained and documented.

5. Once the set of system properties, models and parameters is available, they are combined in a scheme that serves to explore all interactions modeled and predict failure probabilities. Because failures tend to be mainly due to a combination of unfavorable circumstances that may occur in nature, a scheme to predict failure probabilities such as Monte Carlo simulation would be desirable and it could be practical and acceptable. Other probabilistic schemes might be acceptable as well. Indeed, a preferred scheme can not be identified at this time, due to the fluid state of the field of high level waste repository design and analysis.

Sensitivity Analysis

The assembled waste package model or subsystem models could be used preliminarily to perform sensitivity calculations. These calculations are useful in identifying the most important parameters and links, and may help define the data needed to predict an "acceptable" level of uncertainty.

1.4 Purpose and Organization of the Report

This report presents a first attempt at describing how a Probabilistic Reliability Analysis of high level waste packages could be made based on available reliability guidelines. As such it cannot be considered as a comprehensive document, but rather as a focus for further discussion and improvements.

Presented in Chapter 2 are suggested regulatory requirements on the information that would be expected of the applicant in order to substantiate, before the NRC, compliance of the proposed design with 10 CFR 60 performance criteria. Chapter 3 reviews the analyses that would be expected of the applicant, while Chapter 4 presents a simple illustration of waste package reliability analysis. The technique for uncertainty propagation which is discussed and implemented in these chapters is known in the literature as Monte Carlo simulation. As pointed out before, other techniques may be available. Rather than comparing these techniques, our purpose is to show that at least one technique exists. Finally, conclusions and recommendations are provided in Chapter 5.

2. SUGGESTED REQUIREMENTS FOR ON RELIABILITY ANALYSIS

2.1 Information Required For Evaluation Of Reliability

The applicant should submit to the NRC a Safety Analysis Report (SAR) in accordance with the requirements of the Code of Federal Regulations (10 CFR 60.21). The prediction of reliability of the waste package should be part of the SAR.* This report will conform to the guidelines of a Standard Format.

The applicant should strive for clear, concise presentation of the information provided in the SAR. The required information should include:

1. Waste package design configuration and materials specification
2. Conditions that bound the repository environment
3. Material properties of the selected waste package components
4. Failure mode and effects analysis
5. Quantitative reliability analysis of the proposed waste package design
6. Quality assurance procedures

2.1.1 Waste Package Design Configuration and Materials Specification

According to 10 CFR 60, the waste package includes:

(1) The waste form, which consists of the radioactive waste proper and any associated encapsulating or stabilizing materials.
(2) The container, which is the first major sealed enclosure that holds the waste form.

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*If a format and Content Guide for the SAR is issued by the NRC, then the information identified below is to be considered supplementary to the waste package portion.

(3) Overpacks, which consist of any additional vessel receptacle, wrapper, box or other structure, that are both within and an integral part of a waste package and provide additional containment of the waste.

(4) Packing material, which may control the flow of groundwater, condition the chemistry of the groundwater reaching the container or overpack, and retard the transport of radionuclides from the waste after the container is breached.

This constitutes four major barriers. A specific waste package system is considered in Chapter 4 for the purpose of illustration.

In the SAR, the applicant should submit drawings and schematics of the proposed waste package design. Detailed material specifications should be also included.

2.1.2 Environmental Conditions

In the prediction of reliability of the waste package, the applicant should show the extreme range of conditions that bound the environment to which the waste package may be subject throughout its life. This is accomplished by providing ranges of values for the following factors of environmental concern:

- temperature field
- groundwater flow rate, quantity, and chemistry (including pH, Eh, oxygen and hydrogen fugacities)
- radiation field
- pressure and stress fields
- air/steam and other gases composition and flow rate*

These factors influence singly or concurrently all degradation modes of waste package components, as shown in Table 2.1-1.

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*Required only if the repository is located in the unsaturated zone.

Table 2.1-1

Degradation Modes of Waste Package Components

and Relevant Environmental Factors for Reliability Analysis

Waste Package Component	Degradation Mode	Environmental Factor
Primary Waste Form	Leaching	A,B,C,E
	Phase Changes	A,B,C,D
	Fracturing	A,B,C,D,E
Structural Metal Components	Mechanical Failure	A,C,D
	Corrosion	A,B,C,D,E
	Hydrogen Embrittlement	A,B,C,D,E
	Leaching	A,B,C,E
Packing Material	Chemical Failure	A,B,C,E
	Phase Changes	A,B,C,D
	Fracturing	A,B,C,D,E

A - Temperature field

B - Groundwater chemistry

C - Radiation field

D - Pressure and stress fields

E - Gaseous fluids chemistry

2.1.3 Material Properties

In the prediction of waste package reliability, the applicant should list, for each waste package component, material properties necessary to accomplish reliability analysis. These may include original composition and mechanical, chemical and thermal characteristics, and their expected dependence on the repository environmental factors as they change with time. These properties impact on the design functions of each waste package component and constitute an indispensable data base for evaluating performance. For the the sake of illustration, an abridged list of expected properties to be provided by the applicant and the function they impact on is reported in Table 2.1-2 for a generic packing material.

2.1.4 Failure Mode and Effects Analysis

In the SAR, the applicant should list all possible, identified failure modes of each waste package component and their retention or dismissal for further analysis. This preliminary analysis, generally called Failure Mode and Effects Analysis - FMEA, is qualitative in nature[3]. It is expected to result in the reduction of the set of possible failure modes to only those which are relevant under the range of repository conditions identified in Section 2.1.2. This set of significant failure modes will be called design failure modes. In the dismissal of potential failure modes, the applicant should consider the natural variability of environments to which the package will be exposed. The dismissal of any given failure mode should be discussed and documented.

Special forms of the kind shown in Table 2.1-3 are useful for documenting an FMEA. Furthermore, the interrelations between design failures can be summarized by means of event or fault trees. An example of a fault tree for waste package analysis is presented in Figure 2.1-1

2.1.5 Quantitative Reliability Analysis

For each of the design failure modes and for each basic process determining the evolution of environmental conditions and material property

Table 2.1-2
Material Properties of Generic Packing Material
for Reliability Analysis*

Function	Properties
Groundwater Exclusion	Porosity Permeability Hydraulic Conductivity Swelling pressure
Radionuclide Retention or Retardation	Dispersivity Diffusivity Tortuosity Radionuclide Loading Capacity
Mechanical Stability	Elasticity Moduli Compressive Strength Shear Strength
Heat Transfer	Thermal Conductivity Thermal Diffusivity Emissivity Overall Heat Transfer Coefficient**
Resistance to Hydrothermal Alteration	Thermal Expansion Coefficient T-V-P Points for Change of Phase
Groundwater Conditioning	Eh-pH Stability Fields Solubility Limits Sorption with Respect to O_2

* list of properties not intended to be complete.
**under both water saturated and non-saturated conditions.

Table 2.1-3

Exemplary FMEA Documentation for Failure Modes* of a Waste Package Component

Waste Package Component	General Failure Mode	Identified Failure Modes	Design Failure Modes
Waste form container (low carbon steel)	Chemical	Uniform corrosion	Uniform corrosion
		Pitting ''	Pitting ''
		Galvanic ''	Stress corrosion cracking
		Crevice ''	
		Intergranular ''	Hydrogen embrittlement
		Bacterial ''	
		Erosion ''	
		Stress corrosion cracking	
		Hydrogen damage	
		Selective leaching	
	Mechanical	--	--
		--	--
		--	--
		--	
		--	
	etc.		

*List of failure modes not intended to be complete.

Example Fault Tree

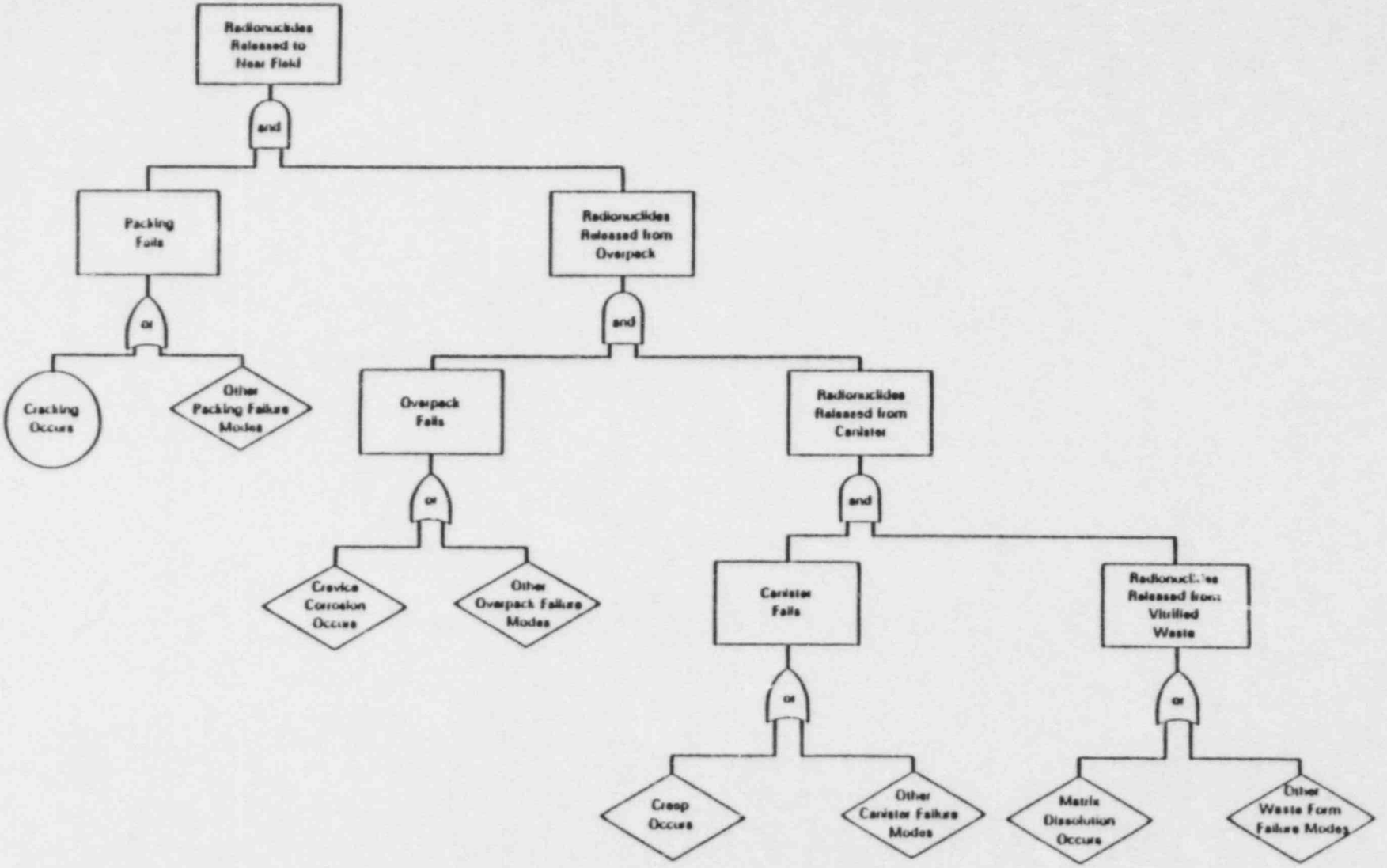

Figure 2.1-1

changes, the applicant should supply predictive equations. For each predictive equation, the applicant should provide the theoretical foundation, experimental verification or other form of validation, and an analysis of the uncertainty of prediction associated with the equation. The uncertainty of the equation with respect to reference data should be established through statistical evaluation of the scatter of data. The uncertainty of the equation with respect to its applicability (model uncertainty) should be established through a survey of expert opinions. In addition, for all the data required for the predictive equation, the applicant should supply detailed probability distributions. The last requirement may be relaxed for some parameters if the applicant has performed a sensitivity analysis which indicates that the overall waste package performance is insensitive to these parameters under expected repository conditions. In general, the degree of rigor with which the probability distributions are developed depends on the application and desired accuracy of the analysis. From this information, a quantitative reliability analysis of the proposed waste package design should be possible.

In order to perform a quantitative reliability analysis of the proposed waste package design, the applicant should combine the various models for design failure modes, material properties changes, and evolution of the waste package environment in a composite model called the performance model. By the use of the performance model and the random variables representing the data and the uncertainty of the individual models used, the applicant should then derive the probability distribution of the times to containment and controlled release failure. A scheme to predict failure probabilities such as a Monte Carlo simulation would be desirable and it is implemented in this document (Chapter 4). Other probabilistic schemes might be acceptable as well. Indeed, a preferred scheme cannot be identified at this time due to the fluid state of high level waste repository design.

2.1.6 Quality Assurance Procedures

In order to provide assurance that the design, construction, and operation of the proposed repository is in conformance with applicable regulatory

requirements and with the design bases specified in the license application, 10 CFR 60 requires that a Quality Assurance Program (QA Program) be established by the applicant.

The QA program should assure confidence in the reported distributions for the material parameters used in the performance model. Indeed, design reliability specifications are an integral component of most good QA programs[6].

3. REVIEW PROCEDURE AND ACCEPTANCE CRITERIA

A definitive selection of a necessary and sufficient set of critical parameters and models of mechanisms, such that their consideration insures completeness of the review of the waste package reliability analysis will not be possible until the waste package designs are defined, because the importance of a given parameter or model depends on its role in the whole system.

There are, however, some basic system parameters and models that can be identified initially and that are expected to form a core of critical items to deserve attention during review. These will occupy the bulk of this section. Other parameters and phenomena not included in this review may become important as the analysis of particular designs matures. They should be included in the licensing review as the developing experience dictates the need.

This section of the report also suggests general guidelines for documenting models. These guidelines complement the NRC position on the subject as codified in NUREG-0856 of December 1981.

3.1 Failure Mode Analysis

The failure mode analysis consists of a description of the mechanisms and processes that are liable to lead to a failure of the system to perform its intended function under the expected repository conditions. It contains in narrative form, the modes of failure considered in the analyses and design failure modes. The interrelations between components failures may be summarized by means of fault or event trees.

The review of the failure mode analysis serves the reliability specialist to define the failures that need to be analyzed further to calculate the reliability of the system.

The acceptability the failure mode analysis depends on the completeness of the phenomena considered in its formulation. There are no practical methods to prove completeness other than a documented record of search and analysis of

alternative failure modes such that repeated detailed review by competent technical persons fails to produce new credible and significant failure modes. Such review should be conducted at a pace that will allow the reviewers to explore alternatives suggested by the review, and should result in documentation of the alternatives considered and dismissed.

3.2 Quantitative Reliability Analysis

In order to calculate the reliability of a waste package design in a geologic repository, a Monte Carlo simulation method can be useful and is adopted in this report. Other methods may also prove to be acceptable.

In the Monte Carlo method one views the parameters of the waste package performance model as random variables with given distribution functions, samples among these with an appropriate technique based on a random number generator approach, and determines performance. The process is repeated several times in order to simulate any combination of parameters or environmental conditions considered possible for the design. When some of the component models have uncertainties in themselves, in the sense that even if the input were known perfectly the output would be uncertain, one accomodates this by introducing in the component model an extra random variable to represent the model uncertainty. Alternatively, in a Monte Carlo simulation a numerical experiment is set up which behaves as much as the actual problem as possible. The modeled process is then observed, and the results are tabulated and treated as if they were the outcome of an experiment. Features of a waste package Monte Carlo reliability calculation are presented in Figure 3.2-1. The technique is illustrated in the worked example reported in Chapter 4.

Acceptability of a Monte Carlo reliability calculation depends on the proper selection of a performance model, numerical inputs, random sampling technique, and algorithms and computer programs. These are reviewed independently as follows.

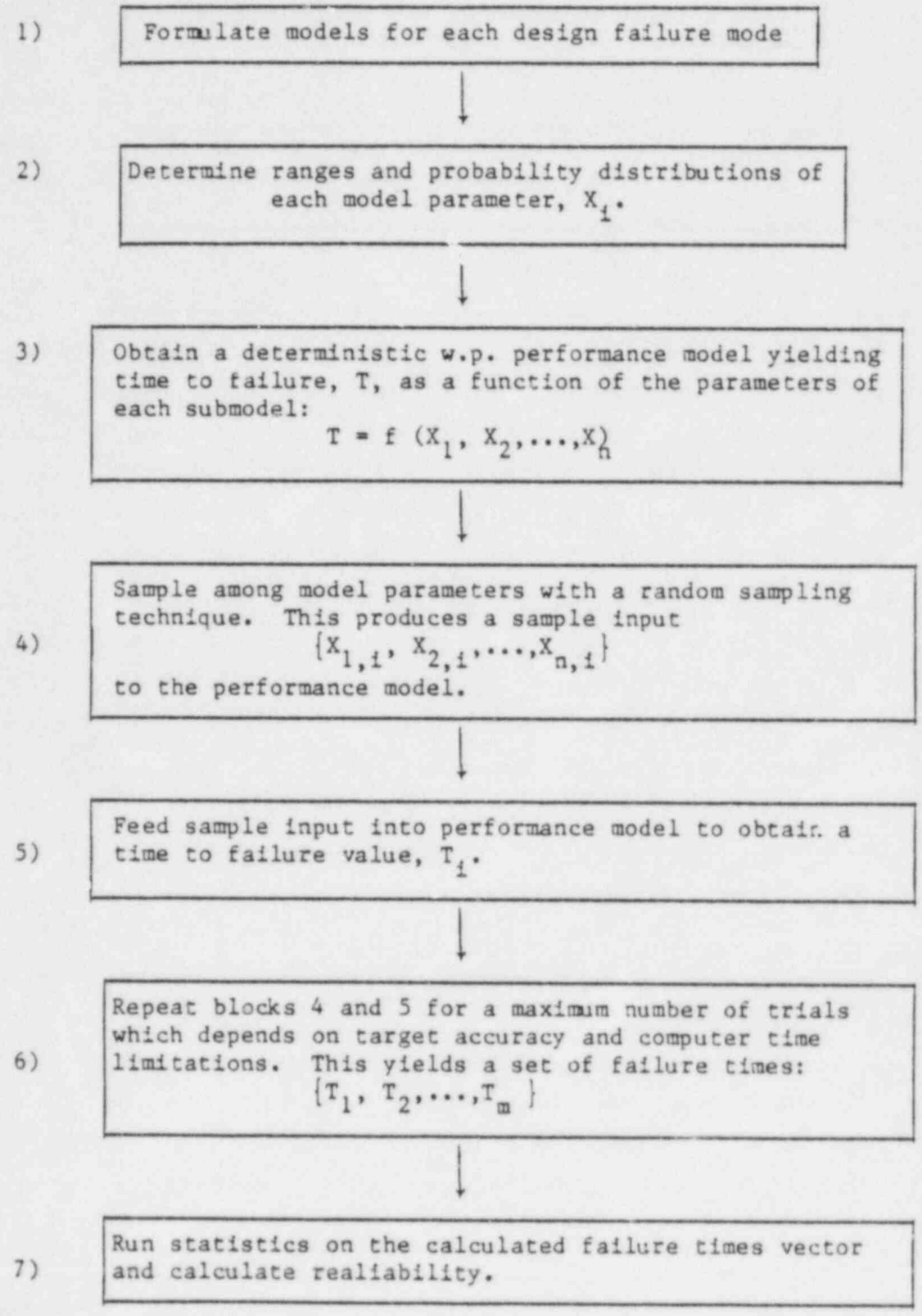

Figure 3.2-1. Monte Carlo simulation principles for waste package reliability analysis.

3.2.1 Performance Model

A waste package performance model will be composed of component models addressing basic functions or processes within the waste package system. The validity of the performance model depends on the completeness with which the individual component models describe all phenomena of importance, and, in final analysis, on their success in predicting experimental results.

In order to insure completeness of the review, the derivation of predictive equations for the purpose of correlation of experimental results should be described in sufficient detail to allow independent verification and reconstruction of the predictive equation by qualified practitioners. For widely used predictive equations in the public domain, e.g., conventional heat transfer correlations, identification of sources and reference to publications is sufficient. For predictive equations developed specifically for evaluation of waste package performance and used in the reliability assessment, the data base used for the derivation of the equation should be provided in tabular form either originally or by reference to published reports. The analysis of the data should include an analysis of correlation between the independent variables, measures of goodness of fit of the regression in the form of significance levels of the estimate of regression coefficients, and analysis of residuals to demonstrate the form of the distribution function of the expected errors.

Models to be used for Monte Carlo simulation will result, for practical reasons, in relatively simple algorithms. For example, temperature calculations will be probably reduced to one-dimensional models to keep computer time within practical limits. In cases where such simplifications are needed, it is stressed that these models will require further validation of the simplifying assumptions by comparison against detailed calculations accepted to serve as benchmarks.

Since the design of high level waste packages is not sufficiently defined to permit a complete specification of the performance model, the following considerations should serve as a guideline. It is expected that a performance model should be composed of the following component models:

- A temperature model able to predict the temperature at any point in the waste package as a function of time.
- A heat source model able to predict the rate of heat generation in the waste as a function of time.
- A radiation model able to predict gamma dose rates in the waste package
- A water flow model able to predict groundwater flow as a function of time, perhaps accounting for temperature gradients.
- A water chemistry model able to predict the parameters of interest such as pH, Eh and salt concentrations as a function of temperature, radiation and time.
- A corrosion model able to predict corrosion rates as a function of temperature, water chemistry and radiation dose rates.
- A mechanical failure model able to predict damage to the canister due to stresses.
- A solubility limited leach model able to predict release rates of radio-isotopes as a function of time, temperature and water chemistry.
- A packing material transport model able to predict concentrations of isotopes as a function of time, water flow, temperature, water chemistry, and radiation field.

3.2.2 Numerical Data and Constants

The basic criterion for acceptance of numerical data to be used in models or correlations is reproducibility. For experimental data, the conditions of the experiment should be stated or referenced such that the results can be reproduced within stated experimental error by a qualified practitioner. For derived data, the results should be computable from the supplied or referenced sources.

All constants and parameters resulting from experimental measurements and used in the analysis of performance or reliability of the package should be presented with an estimate of the error or confidence interval. In the case of experimental data having uncertainties larger than a few percent, an estimate of the expected distribution of errors should be provided. All basic experimental data used for the derivation of models should be provided in a form, such as

tables or references to available publications of numerical data, that will permit that any derived correlation or predictive model used in the analysis of reliability be reconstructed as the need arises during the review. Data in the form of plots are not acceptable for the justification of models unless accompanied by tabulations of the numerical values. References to data in unpublished draft reports and publications are not acceptable.

3.2.3 Random Sampling Technique

Reliability calculations based on Monte Carlo simulation necessitate the repetitive use of the waste package performance model with different values of the input parameters viewed as random variables. Since accuracy improves the larger the number of cases which are analyzed, a conflict exists between accuracy and economy of reliability calculations. This conflict is expected to be resolved by selecting an appropriate technique which samples randomly among the input parameters of the model.

The review should insure that the chosen random sampling technique correctly selects parameter values which reflect the original probability distributions, and that any pair of independent parameters are indeed uncorrelated when selected in small samples. Conversely, in a reliability calculation, total lack of correlation between all parameters may not actually represent the real situation. For example, in the cases of the thermal conductivity and the specific heat of the host rock there may not be a firm functional dependence between them, but they may not be really independent either. Thus, the chosen random sampling technique should have the capability of treating correlation between random variables when needed.

The technique used for the sample calculation of Chapter 4 is known in the literature as the "Latin Hypercube Sampling Plan" (SAND-79-1473; 1980), which produces samples of random variables with rather uniform coverage and controlled correlation. Other sampling techniques may be acceptable as well, provided proper justification be given with reference to the open scientific literature, or, if originally developed, by providing analyses of actual test runs.

3.2.4 Algorithms and Computer Programs

The basic criterion for acceptance of results obtained through the use of algorithms and computer programs shall be independent reproducibility of computed results by a qualified practitioner and disclosure of the method, computer program listings, and details of computation in sufficient detail to allow a completely independent analysis, unless an alternative fully documented computational method exists in the public domain capable with the same data to reproduce the results within the necessary accuracy. This exception serves to protect proprietary methods that may have advantages of speed, accuracy or cost. Further guidance for the content of documentation on computer models to be used in support of a license application for high-level waste disposal is given in NUREG-0856 of December 1981.

4. RELIABILITY ANALYSIS ILLUSTRATION THROUGH MONTE CARLO SIMULATION

4.1 Introduction

To serve as an illustration of Monte Carlo waste package simulation and of techniques which can be used for models formulation, one of the waste package designs described in the Site Characterization Report for the Basalt Waste Isolation Project (DOE/RL82-3) was selected for analysis. This design, henceforth called Sample Design, involves borosilicate glass, a carbon steel canister and a basalt-bentonite packing in horizontal emplacement holes.

This illustration does not attempt to produce a complete analysis but only to show for a few components, how the probability of failure could be derived. The use of simplified descriptive models is illustrated by the thermal and transport models. The development of predictive equations is illustrated for the case of corrosion, where techniques are shown that could be used to justify the model, if appropriate data were available. Techniques to factor in expert opinion in defining models uncertainty and completeness uncertainties are not shown in this illustration. These are discussed in Reference [2].

The analyses in this chapter are included for demonstration purposes only and the NRC neither approves nor disapproves of the specific simplifications and approximations made hereafter. The Commission will review any DOE computer code for acceptability based upon the types of analyses it is to be used for and the data requirements for that code or model.

4.2 Failure Mode and Effects Analysis

For the purpose of this illustration, and without a judgement as to the probability of other failure modes, the only design failure modes of the Sample Design package to be considered are (a) pitting corrosion of the metal canister followed by (b) leaching of the glass and (c) transport of radioisotopes through the packing material. It is further assumed that the packing material is saturated with water and that the chemical composition of the water saturating the packing material is not modified by the effects of ionizing radiation.

4.3 Quantitative Reliability Analysis

In order to perform a quantitative reliability analysis of the Sample Design, a Monte Carlo simulation method is implemented in this chapter according to the operational procedure outlined in Section 3.2.

Following the simplified FMEA of Section 4.2, the adopted performance model consists of the following component models: (a) a temperature model, (b) a canister-corrosion model, and (c) a combined, leaching and radioisotope-migration model. Temperature feeds back on both the other models. In general, however, these models may depend on each other in a complex manner which is not fully explored in this document. For instance, in a more rigorous calculation, the canister-corrosion and leaching-and-migration models should be interrelated to a water-chemistry model which in turn receives inputs from the temperature and ionizing-radiation models. A water chemistry model is not available at this time. Thus, water chemistry is treated here as a set of inputs (with appropriate uncertainty ranges) which feed back on corrosion alone.

The three component models to be used in this illustration are individually obtained in forthcoming subsections. The resulting performance model is combined with the Latin Hypercube random sampling technique in Section 4.4. Results of the reliability analysis are presented in Section 4.5.

4.3.1 Package Temperature Model

In this illustration, the package temperature model serves essentially to predict canister temperature as a function of time, as temperature constitutes an important input to the corrosion model.

Clearly, a rigorous calculation using one of the three-dimensional heat transfer codes such as HEATING6 (ORNL-NUREG-CSD-2; 1982) would be appropriate for the accurate prediction of temperature. However, performing one run of HEATING6 is in itself a substantial computer effort which precludes its use in a performance model to be used in a Monte Carlo simulation. Indeed, as indicated earlier, models for use in a Monte Carlo reliability analysis need to be

simple while retaining sufficient accuracy. Since the derivation and validation of one such model is beyond the scope of this illustration, a plausible model is presented here based on engineering judgement.

In order to derive a simplified model, the three-dimensional heat transfer problem is reduced to two coupled one-dimensional cases encompassing a far field effect and a near field effect. With reference to Figure 4.3-1, the far field of the repository is defined as that portion of the geologic formation where the details of the spatial distribution of the heat sources (waste packages) is unimportant for temperature profiles calculations. The near field is the region in the neighborhood of the packages where the temperature field shows the effects of the individual rows of packages.

Heat transfer in the far field is assumed to take place by conduction, and the temperature profile away from the near field is obtained as a function of time by assuming instantaneous transfer of heat across the near field to the lower boundary of the far field. This initially overestimates the temperature profile away from the source, but it is an increasingly accurate estimate as time goes by. In particular, as it is shown in Appendix B, the temperature in the far field is given as:

$$T_F(t) = \frac{1}{K}\left(\frac{k}{\pi}\right)^{1/2} \sum_{i=1}^{n} \frac{a_i}{\sqrt{\lambda_i}} \Delta(\sqrt{\lambda_i t}) + T_o \qquad (4.3\text{-}1)$$

where k and K represent the thermal diffusivity and conductivity in the far field, respectively; a_i, λ_i empirical coefficients in the expression for the decay heat per unit area when this is fitted to an expression of the form:

$$f(t) = \sum_{i=1}^{n} a_i \exp(-\lambda_i t); \qquad (4.3\text{-}2)$$

$\Delta(x)$ is the Dawson's integral defined as follows:

$$\Delta(x) = \exp(-x^2) \cdot \int_0^x \exp(+t^2)\, dt \; ; \qquad (4.3\text{-}3)$$

and T_o is the geothermal, background temperature before emplacement of the waste.

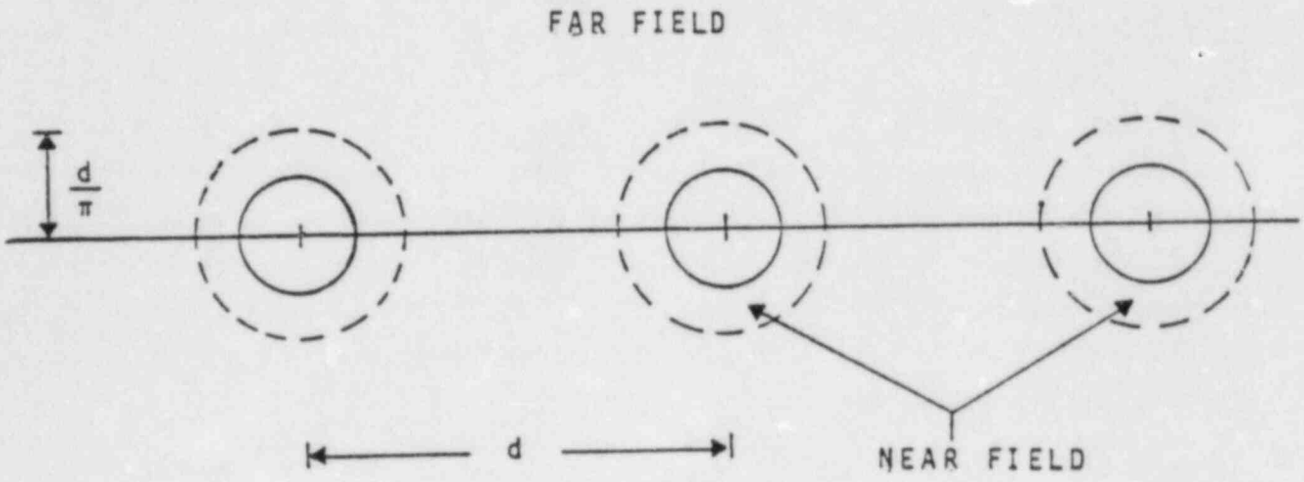

Figure 4.3-1. Schematic Description of the near and far field of the repository.

According to the hypothesis of instantaneous heat transfer in the near field, heat conduction is treated here as a sequence of steady-state states characterized by a temperature drop across the near field:

$$\Delta T = T_N - T_F \tag{4.3-4}$$

where T_F is given by Eq. (4.3-1). An expression for this "steady state" temperature drop can be obtained by considering conduction through concentric cylinders representing the waste package plus a suitable portion of the host rock. The selection of the portion of the rock that needs to be incorporated in the near field model to obtain the best approximation is not trivial, and should be determined by comparison of results with detailed analysis. For the purpose of illustration, the outer diameter of the equivalent rock shell is taken such that the outer surface of the shell corresponding to a waste package is equal to the horizontal surface (floor) of the repository. The outer diameter of the equivalent rock shell could also have been selected as equal to the distance between rows of packages. On the basis of engineering judgement and for the purpose of illustration, the first assumption was selected. Thus, the radius, R, of the outermost cylinder is related to the distance, d, between emplacement holes through the expression:

$$R = d/\pi \tag{4.3-5}$$

and the temperature at the repository floor is:

$$T_N = T_F(t) + \Delta T \tag{4.3-6}$$

where ΔT is obtained as a sum of terms of the form:

$$\Delta T = \frac{P}{2\pi KL} \ln (D_2/D_1) \tag{4.3-7}$$

representing the steady-state temperature drop between two concentrical cylindrical shells of diameter D_1 and D_2 respectively, for each of the components of the waste package and for the equivalent rock shell.

The model used here for illustration purposes has made use of several simplifying assumptions which should have required extensive evaluation for an actual application and would probably require extensive changes. Indeed, justification of the models used in the reliability analysis will be an important and significant task for the analyst. In this particular model assumptions include: the rock has temperature independent properties, all the packages have equal heat generation rates, the repository has infinite dimensions, the effect of the earth surface is neglected, and the potential effects due to water evaporation are neglected.

The details of this simplified model are discussed in Appendix B.

4.3.2 Canister Corrosion Model

As indicated by the simple FMEA analysis of Section 4.2, the only design failure mode considered for the waste form canister is pitting corrosion, of which a model is developed hereafter. Other failure modes could be analyzed as well through the techniques presented in this section.

The model to be developed for this illustration assumes that pitting corrosion differs from uniform corrosion through a multiplicative factor. Thus, uniform corrosion data are analyzed first in Section 4.3.2.1 and fitted in Section 4.3.2.2 to a predictive equation dependent on a small number of parameters whose significance to the corrosion process is statistically calculated. Statistical uncertainty of the prediction is taken into account in Section 4.3.2.3 through a multiplicative uncertainty factor derived from statistical considerations about the internal consistency of the data. Both the model uncertainty factor with respect to the reference data and the model parameters are viewed as random variables with appropriate ranges and distributions. A pitting factor, viewed as a random variable is then calculated in Section 4.3.2.4, and a pitting corrosion model is assembled together in Section 4.3.2.5.

4.3.2.1 Reference Data Base

In order to formulate a predictive equation for the corrosion rate on empirical grounds, a reference experimental data base should be used which covers the spectrum of conditions expected in the repository during the period of interest. In other words, the population sampled by the experimental data should fairly reflect the population of conditions for which the prediction is needed. Such a data base is not available at present.

For the purposes of illustration, reference is made here to the collection of data used by Westinghouse in AESD-TME-3113 for steel. These data have been assembled in a consistent form in Table 4.3-1. In this table, originally reported uniform corrosion rates have been converted to uniform corrosion depth by thorough multiplication by the duration of the experiment, which is also recorded. Data originally reported as "Average Corrosion Rate" have been interpreted as uniform corrosion rate. When the results were described as corresponding to oxic or anoxic conditions without specifying the oxygen content, oxygen concentration values of 0.1 and 3 ppm have been assumed respectively. For brine and seawater, the chlorine ion concentration has been assumed to be 200,000 and 20,000 ppm respectively. All the steel compositions and water chemistries have been lumped together into a single population for the purposes of the forthcoming analysis. Thus, Table 4.3-1 constitutes a data base of 55 cases spanning a broad spectrum of temperatures and chlorine and oxygen concentrations. The data base has many shortcomings, of which the most important are want of long term cases and inhomogeneity of the sample. In addition, a substantial correlation exists in these data. For example, all of the long term cases were observed in low temperature oxic conditions at the Gatun Lake, Panama, in fresh water.

4.3.2.2 Uniform Corrosion

The selected mathematical form of the expression for the depth of uniform corrosion is

$$U_C = K \cdot \exp\left(\frac{a}{T}\right) \; O^b \cdot Cl^c \cdot t^n \qquad (4.3\text{-}8)$$

Table 4.3-1 (Continued)
Steel Corrosion Data Base

Material	Temp °C	Chlorine ppm	Oxygen ppm	Unit Corrosion mm	Pitting Corrosion mm	Time years
Steel 1080	250	18980	0.03	0.0338	NA	0.083
Steel A570	250	30000	0.01	0.0741	NA	0.083
Steel A53B	250	30000	0.01	0.0508	NA	0.083
Steel C75	250	30000	0.01	0.0338	NA	0.083
Steel 1010	250	30000	0.01	0.0804	NA	0.083
Steel A570	250	60000	0.01	0.0908	NA	0.083
Steel A53B	250	60000	0.01	0.0761	NA	0.083
Steel C75	250	60000	0.01	0.0148	NA	0.083
Steel 1010	250	60000	0.01	0.0866	NA	0.083
Steel A570	250	120000	0.01	0.2325	NA	0.083
Steel A53B	250	120000	0.01	0.2308	NA	0.083
Steel A53B	250	120000	0.01	0.2650	NA	0.083
Steel C75	250	120000	0.01	0.1691	NA	0.083
Steel 1010	250	120000	0.01	0.2875	NA	0.083
Steel CortenA	250	145833	0.03	0.0042	NA	0.083
Steel 1018	250	145833	0.03	0.0063	NA	0.083
Steel CortenA	250	159416	0.03	0.0741	NA	0.083
Steel 1018	250	159416	0.03	0.1417	NA	0.083
Cast Iron 22-8	250	159416	1.0	0.1058	NA	0.083
Cast Iron 22-8	250	159416	1.0	0.1483	NA	0.083
Cast Steel 27C	25	70	3.0	0.21	.76	1.00
Cast Steel 27C	25	70	3.0	0.30	NA	2.00
Cast Steel 27C	25	70	3.0	0.36	NA	4.00
Cast Steel 27C	25	70	3.0	0.48	1.70	8.00
Cast Steel 27C	25	70	3.0	0.66	2.49	16.00
Gray Iron 3.2	25	70	3.0	0.18	1.32	1.00
Gray Iron 3.2	25	70	3.0	0.30	NA	2.00
Gray Iron 3.2	25	70	3.0	0.38	NA	4.00
Gray Iron 3.2	25	70	3.0	0.58	2.69	8.00
Gray Iron 3.2	25	70	3.0	0.84	2.74	16.00

Note: NA - not available.

where

U_C = Uniform Corrosion Depth [mm],
T = Absolute Temperature [K],
O = Oxygen Concentration [ppm],
Cl = Chlorine Concentration [ppm],
t = Time [years],
K = Uniform corrosion factor.

For the purpose of data fitting, Eq. (4.3-8) is first linearized through a logarithmic transformation, using the natural log, and by using an inverse transformation on the absolute temperature. Then, in order to make sure that the chosen variables in Eq. (4.3-8) are indeed independent of each other, a correlation matrix is computed between the transformed variables in terms of the reference data base [19]. The correlation matrix is reported in Table 4.3-2.

A substantial correlation exists between time and temperature, reflecting the fact that all of the data for long times corresponds to 25°C temperatures. The correlation between oxygen and chlorine levels is also substantial.

In order to illustrate the effect of the strong correlations between some of the variables in Eq. (4.3-8), a multivariate regression of the transformed data has been performed using the program REGRESSION of the Statistic Package for the Social Sciences [21] (SPSS), a general purpose collection of statistical programs. The results of the regression are presented in Table 4.3-3.

Table 4.3-2

	INVTEMP	LCHLOR	LOXYG	LUCORR	LTIME
INVTEMP	1.0000	0.1582	0.2808	0.0145	0.7447
LCHLOR	0.1582	1.0000	-0.5221	0.7314	0.0368
LOXIG	0.2808	-0.5221	1.0000	-0.2724	0.3525
LUCORR	0.0145	0.7314	-0.2724	1.0000	0.2265
LTIME	0.7447	0.0368	0.3525	0.2265	1.0000

Table 4.3-3

Variable	Regression Coeff.	Standard Error
Ln (Time)	1.658	0.223
Ln (Oxygen)	0.114	0.101
(1/Temp)	-1625	0.557
Ln (Chlorine)	0.466	0.0646
Intercept	0.764	0.863

The effects of correlation between the data leads to a power of time equal to 1.658 which implies an accelerating rate of corrosion with time. A result which is contrary to experience. Thus, even if, as a fit of the data, the regression reduces the variance to 37% of the original, it leads to misleading results as a method of extrapolating corrosion to longer times.

In an effort to reduce the effects of correlation among the data, the last 10 data points, representing long term experiments, are separated and the two groups of data are analyzed independently. Since the data of this second subset of 10 points contain only time, uniform corrosion, and pitting corrosion as variables, they are used to derive the time dependence. The results of a regression between logarithm of uniform corrosion and logarithm of time gives a coefficient of regression of 0.4689 with a standard error of 0.0339. If the normality assumption is made such that the 0.001 quantile corresponds to 3.09 standard deviations, the range can be estimated as 0.4689 ± 0.1047= 0.3639 to 0.5736. This estimate of the range of the exponent of time is based on corrosion of steel and gray iron in fresh water at 25°C in the Gatun Lake and it does not necessarily represent the uncertainties of applicability of the data to repository conditions. However, to proceed with the illustration, that range is adopted.

Once the time dependence is obtained, the fit of the data for the other coefficients is continued by considering the new transformed dependent variable defined as

$$LL = \text{Ln}\,(U_c) - 0.4689\ \text{Ln}\,(t) \qquad (4.3\text{-}9)$$

Table 4.3-4

	INVTEMP	LCHLOR	LOXYG	LL
INVTEMP	1.0000	0.1582	0.2808	-0.0822
LCHLOR	0.1582	1.0000	-0.5221	0.7423
LOXYG	0.2808	-0.5221	1.0000	-0.3242
LL	-0.0822	0.7423	-0.3242	1.0000

The Pearson correlation matrix for the first group data is given in Table 4.3-4. The strong correlation between the oxygen and chlorine is expected to affect the results. Table 4.3-4 shows that temperature is very weakly correlated with the new dependent variable, LL, and hence with the depth of uniform corrosion.

A regression of LL against the inverse of the temperature and the logarithms of the oxygen and chlorine is shown in Table 4.3-5.

From this analysis of the data, the following predictive equation is derived:

$$U_C = e^{-4.148} \; t^{0.469} \; e^{-(\frac{1402}{T})} \; Cl^{0.543} \; O^{0.2}$$

$$= 0.0158 \; t^{0.469} \; e^{-(\frac{1402}{T})} \; Cl^{0.543} \; O^{0.2} \qquad (4.3\text{-}10)$$

Table 4.3-5

Variable	Regression Coeff.	Standard Error
Ln (chlorine)	0.543	0.072
Ln (oxygen)	0.200	0.107
(1/Temp)	-1402	517
intercept	-4.148	1.074

Since the independent variables are dimensional numbers which may take large values and the exponents have been truncated, the errors introduced by the truncation are compensated by adjusting the uniform corrosion factor to reduce to zero the mean of the logarithm of the residuals. The resulting predictive equation is

$$U_C = 0.03725\ t^{0.469}\ e^{-\left(\frac{1402}{T}\right)}\ Cl^{0.543}\ O^{0.2} \qquad (4.3\text{-}11)$$

4.3.2.3 Statistical Uncertainty of the Uniform Corrosion Model

If the original data were representative of the actual conditions present in the repository, then a test of conformity of the model with the data would serve to demonstrate the uncertainties of prediction. However, in this illustration, the data used for the formulation of the model is not homogeneous and does not cover the range of conditions found in the repository. In that case the uncertainty of the model would not be reflected accurately by a measure of conformity such as the standard deviation of residuals.

For the purposes of illustration, and since it is expected that the data used for the justification of the corrosion model used in an actual analysis would really be representative of the actual conditions, the standard deviation of residuals is treated as the measure of errors of the model.

In order to test Eq. (4.3-11) against the original data and calculate the uncertainty of the model, the residuals of the fit of Eq. (4.3-11) to the data are computed and analyzed. To accomodate the wide range of the data, the residuals are taken as the difference between the natural logarithm of the observed uniform penetration depth minus the natural logarithm of the predicted penetration depth. Ultimately this will yield a multiplicative adjustment factor representing the uncertainty of Eq. (4.3-11) in reproducing the actual data. The statistical techniques used hereafter can be found in standard textbooks such as References 18 and 19.

Table 4.3-6 shows the case number, the material identifier, the natural logarithm of the uniform corrosion depth observed, the natural logarithm of the predicted uniform corrosion depth and the difference or residual between the logarithms of the observed and predicted uniform penetration depths. Inspection of the residuals shows that the cases 46 to 55 which correspond to the data taken in the Gatun Lake are highly underpredicted. In general, when data from different sources are grouped together, as is done in this illustration, the homogeneity of the resulting sample should be tested by an analysis of variance of the residuals. In this case, the difference is such that simple inspection shows that the Gatun Lake data is different from the rest.

In order to show the distribution of the residuals, the cumulative distribution of residuals is plotted on normal probability paper to test for normality. Figure 4.3-2 shows the plot of the normalized residuals to the calculated standard deviation of 2.109. The diagonal line represents a perfect normal distribution, and the plot of an empirical distribution from a sample from a normally distributed population is expected to show a random scatter about this line. The larger the sample, the less scatter the points will have.

In the plot, one can clearly identify the group of the Gatun Lake data at about +1.8 standard deviations. The data shows systematic trends for the non Gatun Lake data which comes from the known lack of homogeneity of the data.

To continue with the illustration, and disregarding the evidence of the normal probability paper plot, the data are tested for the hypothesis that the distribution of residuals is normal. For this test, the empirical cumulative probability distribution is computed and it is compared with the assumed cumulative distribution. The statistic used is the analog of the Kolmogorov-Smirnov test as described by Lilliefors[22]. In this test, the empirical cumulative distribution, in this case normalized, is compared with the assumed distribution in the hypothesis testing, and the maximum of the absolute vertical difference is recorded as the statistic. Table 4.3-7 shows the results of intermediate steps of the Kolmogorov-Smirnov test. The residuals are normalized to standard deviation one and sorted in increasing order. The first column shows the case number in the data base to which the point corresponds.

Table 4.3-6 Table of Residuals

CASE	MATERIAL	LOG U.CORR	LOG P.U. CORR	DIFFERENCE
1	1018Steel	-1.9661	-0.97071	-0.99540
2	1018Steel	-3.38140	-2.22102	-1.16038
3	1018Steel	-0.52763	-0.29047	-0.23716
4	1018Steel	-0.09431	-1.54078	1.44647
5	1018Steel	-5.14990	-2.37749	-2.77241
6	1018Steel	-5.99147	-2.99472	-2.99674
7	27C Steel	-1.66073	-2.39749	0.73675
8	Cast Iron	-2.24432	-0.97071	-1.27360
9	Cast Iron	-1.91054	-0.97071	-0.93983
10	Gray Cast	-1.38629	-2.39749	1.01119
11	CastI 80-7	-6.26590	-5.01386	-1.25204
12	CastI 80-7	-6.16582	-5.01386	-1.15195
13	CastI 22-8	-4.11659	-5.01386	0.89727
14	CastI 22-8	-6.11930	-5.01386	-1.10543
15	CastI 142-12	-7.01312	-5.01386	-1.99925
16	CastI 142-12	-6.03229	-5.01386	-1.01842
17	CastI 166-3	-7.13090	-5.01386	-2.11703
18	CastI 166-3	-6.21461	-5.01386	-1.20074
19	CastI 136-04	-6.26590	-5.01386	-1.25204
20	CastI 136-04	-5.99147	-5.01396	-0.97760
21	Steel A570	-3.67301	-3.33529	-0.33772
22	Steel A53B	-3.76360	-3.33529	-0.42831
23	Steel C75	-3.95807	-3.33529	-0.62278
24	Steel 1010	-3.51611	-3.33529	-0.18132
25	Steel CortemA	-4.08044	-2.49024	-1.59021
26	Steel 1080	-3.38730	-2.49024	-0.89706
27	Steel A570	-2.60234	-2.46137	-0.14097
28	Steel A53B	-2.97986	-2.46137	-0.51849
29	Steel C75	-3.38730	-2.46137	-0.92593
30	Steel 1010	-2.52074	-2.46137	-0.05938
31	Steel A570	-2.39910	-2.08499	-0.31411
32	Steel A53B	-2.57571	-2.08499	-0.49072
33	Steel C75	-4.21313	-2.08499	-2.12814
34	Steel 1010	-2.44646	-2.08499	-0.36147
35	Steel A570	-1.45887	-1.70861	0.24974
36	Steel A53B	-1.46620	-1.70861	0.24240
37	Steel A53B	-1.32803	-1.70861	0.38058
38	Steel C75	-1.77727	-1.70861	-0.06866
39	Steel 010	-1.24653	-1.70861	0.46208
40	Steel CortemA	-5.47267	-1.38302	-4.08965
41	Steel 1018	-5.06721	-1.38302	-3.68419
42	Steel CortemA	-2.60234	-1.33466	-1.26768
43	Steel 1018	-1.95404	-1.33466	-0.61938
44	Cast Iron 22-8	-2.24621	-0.63335	-1.61286
45	Cast Iron 22-8	-1.90852	-0.63335	-1.27517
46	Cast Steel 27C	-1.56065	-5.46815	3.90750
47	Cast Steel 27C	-1.20397	-5.14306	3.93909
48	Cast Steel 27C	-1.02165	-4.81797	3.79632
49	Cast Steel 27C	-0.73397	-4.49289	3.75892
50	Cast Steel 27C	-0.41552	-4.16780	3.75229
51	Gray Iron 3.2	-1.71480	-5.46815	3.75335
52	Gray Iron 3.2	-1.20397	-5.14306	3.93909
53	Gray Iron 3.2	-0.96758	-4.81797	3.85039
54	Gray Iron 3.2	-0.54473	-4.49289	3.94816
55	Gray Iron 3.2	-0.17435	-4.16780	3.99345

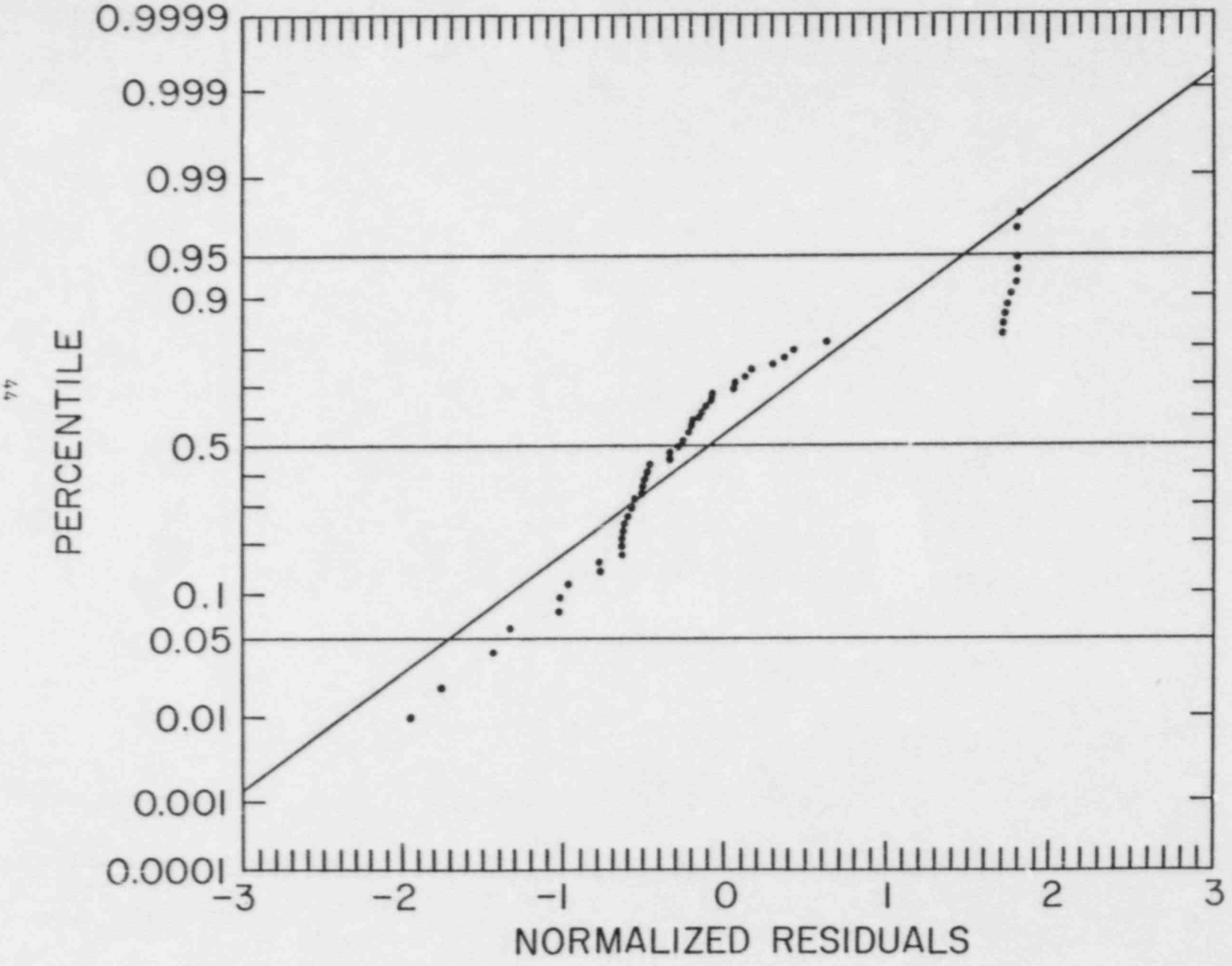
0.9999
0.999
0.99
0.95
0.9
0.5
0.1
0.05
0.01
0.001
0.0001
PERCENTILE
-3
-2
-1
0
1
2
3
NORMALIZED RESIDUALS

Table 4.3-7 Kolmogorov-Smirnov Test

CASE#	RESIDUAL	PROBABILITY EMPIRICAL	PROBABILITY ASSUMED
40	-1.93910	0.02727	0.02625
41	-1.74685	0.03636	0.04033
6	-1.42090	0.05455	0.07767
5	-1.31453	0.07273	0.09432
33	-1.00906	0.09091	0.15647
17	-1.00379	0.10909	0.15773
15	-0.94794	0.12727	0.17157
44	-0.76474	0.14545	0.22222
25	-0.75400	0.16364	0.22543
45	-0.60462	0.18182	0.27272
8	-0.60388	0.20000	0.27297
42	-0.60107	0.21818	0.27391
11	-0.59366	0.23636	0.27638
19	-0.59366	0.25455	0.27638
18	-0.56933	0.27273	0.28458
2	-0.55020	0.29091	0.29110
12	-0.54620	0.30909	0.29247
14	-0.52414	0.32727	0.30010
16	-0.48289	0.34545	0.31460
1	-0.47197	0.36364	0.31848
20	-0.46353	0.38182	0.32150
9	-0.44562	0.40000	0.32794
29	-0.43903	0.41818	0.33033
26	-0.42534	0.43636	0.33530
23	-0.29529	0.45455	0.38389
43	-0.29368	0.47273	0.38450
28	-0.24585	0.49091	0.40290
32	-0.23268	0.50909	0.40800
22	-0.20309	0.52727	0.41953
34	-0.17140	0.54545	0.43195
21	-0.16013	0.56364	0.43638
31	-0.14894	0.58182	0.44079
3	-0.11246	0.60000	0.45522
24	-0.08598	0.61818	0.46573
27	-0.06685	0.63636	0.47334
38	-0.03256	0.65455	0.48701
30	-0.02816	0.67273	0.48876
36	0.11493	0.69091	0.54576
35	0.11841	0.70909	0.54714
37	0.18044	0.72727	0.57161
39	0.21908	0.74545	0.58671
7	0.34932	0.76364	0.63657
13	0.42543	0.78182	0.66473
10	0.47945	0.80000	0.68418
4	0.68583	0.81818	0.75358
50	1.77912	0.83636	0.96239
51	1.77963	0.85455	0.96243
49	1.78227	0.87273	0.96264
48	1.80000	0.89091	0.96407
53	1.82564	0.90909	0.96604
46	1.85272	0.92727	0.96803
47	1.86769	0.94545	0.96909
52	1.86769	0.96364	0.96909
54	1.87200	0.98182	0.96939
55	1.89347	0.99091	0.97085

Kolmogorov-Smirnov Statistic = .183965 Case # = 30

The second column shows the normalized residual. The third column shows the empirical cumulative probability values. The values at both ends are adjusted to the average of the corresponding two extreme values to avoid the problem of probability zero or one. The last column is the quantile of the normal probability distribution which correspond to the argument in the second column. For example, on the row corresponding to case #7, the residual is positive and equal to .34 standard deviations and 76% of the cases have smaller (in the algebraic sense) values. A normal distribution would have 64% of the cases below .34 standard deviations. The maximum absolute value of the difference corresponds to case 30 and is equal to 0.1839 which is the statistic of interest. This statistic can not be interpreted on the basis of the tables of critical values for the classical Kolmogorov-Smirnov statistic because the parameters of the assumed distribution are determined from the sample itself. The critical values determined by numerical calculation by Lilliefors should be used. For 99% confidence level, the critical value given is

$$\frac{1.031}{\sqrt{n}}$$

Since the sample size n is 55, the critical value is 0.1390, therefore we must reject the hypothesis of normality. The test can be interpreted as indicating that the chance of a sample of 55 cases from a normal distribution giving a deviation larger than 0.1390 is less than 1%. However, to continue with the illustration, the assumption will be made that the residuals are distributed normally with zero mean and standard deviation equal to 2.109.

The statistical uncertainty in the prediction of uniform corrosion depth derived from internal consistency of the sample can be represented by a factor which is (on the basis of the above assumption) lognormally distributed. Since the natural logarithm of this factor has an estimated standard deviation of 2.109 the quantiles for 0.001 and 0.999 can be obtained from the table of quantiles of the normal distribution as

$$\exp(-2.109 \times 3.09) \text{ and } \exp(2.109 \times 3.09)$$

or

0.00147 to 676

The resulting predictive equation for uniform corrosion is then

$$U_C = 0.03725\ t^{0.469}\ e^{\left(\frac{-1402}{T}\right)}\ Cl^{0.543}\ O^{0.2}\ \delta \qquad (4.3\text{-}12)$$

where δ is a random variable lognormally distributed with (0.001,0.999) range of (0.00147 to 676).

4.3.2.4 Pitting Corrosion Factor

If data are available which cover the range of conditions to be expected in the application, the ratio between the depth of penetration of pits to the depth of uniform corrosion can be determined from a regression on the data. If the quality of the data available warrants it, the distribution of the depth of pitting should be corrected by the use of extreme value theory.[23]

The only sample data used for this illustration are those of the Gatun Lake, which do not cover anoxic, high chlorine or high temperature conditions. However, for the sake of illustration, a regression of the pit depth vs. uniform corrosion was made using a program from the Statistic Package for the Social Sciences[21]. The resulting regression coefficient result is 2.89 at a significance level of 0.53% and the 95% confidence interval is (1.12, 4.67).

In order to assign a distribution to the ratio of pitting penetration to uniform corrosion depth in the standard format adopted in this methodology, as a range corresponding to the 0.001 and 0.999 quantiles, the assumption is made that the distribution is normal and therefore the 95% limits correspond to 1.96 sigma, at a 3.09 sigma level the range is:

$$2.89 + (4.67 - 2.89)\ \frac{3.09}{1.96} = 5.69$$

$$2.89 - (4.67 - 2.89)\ \frac{3.09}{1.96} = 0.09$$

The same results would have been obtained using the lower value of the confidence interval.

Physically, the ratio of pitting to uniform penetration can not be less than one. Thus the pitting factor is assumed to be distributed between 1 and 6. If the data used were significant and ample enough to determine the shape of the distribution, or if the normality of the distribution where justified on a theoretical basis, then a normal distribution with these parameters would be used. However, since only six points are available and this hardly justifies the wings of the distribution, the assumption of normality is not retained and for the purpose of this illustration, the uncertainty in the ratio of pitting to uniform penetration is arbitrarily represented by a uniform distribution.

4.3.2.5 Pitting Corrosion Model

From the above analysis, the pitting corrosion model can be based on the uniform corrosion model through a pitting corrosion factor, yielding:

$$P_c = K_p \cdot 0.03725\ t^{0.469} \exp\left(\frac{-1402}{T}\right) Cl^{0.543}\ O^{0.2}\ \delta \qquad (4.3\text{-}13)$$

where

P_c = Pitting Corrosion Depth [mm]

K_p = Pitting Corrosion factor, uniform distribution (1 to 6)

This model would serve for prediction over the range of times covered by the data. However, the model is to be used for extrapolation to longer times, and the effect of the uncertainty of the exponent of time factor for times of the order of 1000 years needs to be accounted. Therefore, since the range of the exponent of time has been estimated as (0.3639 to 0.5736) in the final model, the exponent of the time is taken as a random number with normal distribution and that range with quantiles (0.001, 0.999).

4.3.2.6 Rate Model for Pitting Corrosion

The rate of pitting corrosion can be obtained upon deriving Eq. (4.3-13) with respect to time. In particular, by considerations of the previous sections the equation for the rate of pitting corrosion reads as:

$$R_p = K_p\ 0.0372\ n\ t^{n-1} \exp\left(\frac{-1402}{T}\right) Cl^{0.543}\ O^{0.2}\ \delta$$

where

R_p = Rate of Pitting Corrosion [mm/year]

K_p = Pitting factor, uniform (1,6)

n = Exponent of time, normal (0.3639, 0.5736)

δ = Statistical uncertainty in uniform corrosion, lognormal (0.00147,676)

Equation (4.3-14) factors in the statistical uncertainty of the model with respect to the reference data. Based on consensus opinion of experts, the parameter δ could be redefined to include in addition to the statistical uncertainty, which reflects the accuracy of the fit to the reference data, also the uncertainty resulting from the judged adequacy of the model to actual field situations.

4.3.3 Leaching Model

General Considerations

Several reactions can occur between aqueous solutions and radioactive waste forms. The resulting, overall reaction is termed "leaching." Leach rates, i.e., the rates at which radionuclides pass from the solid waste form into the contacting aqueous solution, constitute the source term to all radionuclide hydrogeological transport models.

Several parameters and factors have been found to influence leaching.[7,8] Existing information indicates that major aspects of the long-term leaching behavior will be waste-package design dependent. Indeed, the release of species from a solid to a liquid is controlled by mechanisms involving both solid and solution species. Thus, corrosion products from the canister, overpack materials properties, aging of the waste form, thermal loading, flow rate, etc., all may make major contributions in controlling the long-term leaching behavior. Little or no data exist regarding leaching of candidate nuclear waste forms in the presence of accurate chemical compositions reflecting site specific groundwaters and appropriate waste package rates from rather idealized experimental conditions to the actual repository.

4.3.3.1 Model Formulation

At present, of all major variables influencing leaching, temperature is the only one, with the exception of time, which can be predicted with some degree of confidence. This suggests formulating a leach model which accounts for time and temperature effects only. The influence of other major variables, e.g., groundwater chemistry, aging of the waste form, etc., is lumped in the uncertainties associated with the selected model parameters. If $L_o(t)$ denotes the radionuclide leach rate from the primary waste form, as it is extrapolated from short-term leaching experiments, a generic leaching model in terms of time- and temperature-dependent effects is expressible as follows:

$$L_o(t) = f(t,T), \tag{4.3-15}$$

where $f(t,T)$ is a generic function as yet to be determined. The function $f(t,T)$ has the following properties:

$$\left.\frac{\partial f}{\partial t}\right|_T < 0, \tag{4.3-16}$$

and

$$\left.\frac{\partial f}{\partial T}\right|_t > 0, \tag{4.3-17}$$

indicating, respectively, that leaching is not a self-accelerating process under the assumed radionuclide release scenario, and that leach rates increase monotonically with the temperature of the system.

For designs in which the packing material restricts water flow around a breached canister, a postulated source term represented by a near stagnant, saturated solution seems reasonable. The closest experimental condition to this situation is realized in leaching tests performed under low flow or static conditions within the temperature range expected to exist during the containment period. Low flow leach data for PNL 76-68 glass, the candidate nuclear waste form for commercial high-level waste, are available within the temperature range 25°C to 75°C only[9]. Thus, the only relevant data are those obtained by Westsik and Peters[10] under static conditions within the temperature range 25°C to 250°C in deionized water. These data are also

interesting because they do not show approach to saturation in the temperature range 75°C to 250°C, and the resulting correlation expression for the leach rate:

$$L_o(t) = n(T)\, K(T)\, t^{n(T)-1} \qquad 0 < n(T) \leq 1 \qquad (4.3\text{-}18)$$

should not depend on the parameter SA/V, the solid surface area-to-solution volume ratio.

Eq. (4.3-18) has been used before for waste package analysis calculations[11], and it constitutes the reference leaching model for the present analysis. In particular, the parameter K shows an Arrhenius dependence on temperature, while the parameter n is approximately constant over the range 50°C to 250°C[10,11,12]. Distributions and ranges of these parameters with respect to the data of Westsik and Peters are described in Reference [11]. In actual repository conditions the parameter n may vary with time, reflecting the complex dependence of leaching on the physical and chemical properties of the waste package and groundwater system. Indeed, one expects n to be approximately zero for leaching under near-saturation conditions, and n=1 far from saturation. Thus all uncertainty regarding the effect on leaching of the evolution of the waste package-groundwater system can be lumped into the parameter n.

For the undisturbed repository release scenario, one can propose the following adaptation of Eq. (4.3-18):

$$L_o(t) = n \cdot K(T(t=0)) \cdot t^{n-1} \qquad 0 < n \leq 1, \qquad (4.3\text{-}19a)$$

where the parameter n should be given a uniform distribution of values between n=0 and n=1, and the distribution of the parameter K reflects the initial spread of leaching rates with temperature. In particular, following Reference [11], the parameter K is expressed here as:

$$K(T) = 10^{z} \cdot 10^{(x - y/T)}, \qquad T=T(0), \qquad (4.3\text{-}19b)$$

where z is uniformly distributed between -0.4 and 0.4, x equals 3.18, and y is equal to 2424.22.

Equation (4.3-19) should be regarded as only a tenuous extrapolation of short-term leaching data from rather idealized systems to the actual repository. Better models and better data should be used as they become available. In particular, the new models should factor in the dependence of leaching on solubility limits.

4.3.4 Dispersion Model

4.3.4.1 General Considerations

The two primary mechanisms controlling the transport of radionuclides within the overpack materials are dispersion and convection of solubilized species within the aqueous phase. These mechanisms result in a radionuclide flux, $\underline{J}_g$, given by the expression:

$$\underline{J}_g = - D^* \varepsilon \underline{\nabla} C_w + \underline{u}^* / C_w, \qquad (4.3\text{-}20)$$

where:

D^* - dispersion tensor; [cm^2/yr],
ε - effective porosity of the packing material,
C_w - concentration of the given radionuclide in the aqueous phase; [cm^{-3}],
$\underline{u}^*$ - effective pore water velocity; [cm/yr].

The migration of radioactive species within the packing materials is retarded by sorption-desorption reactions between the aqueous and solid phases, provided the kinetics of the sorption reaction are fast enough compared to radionuclides travel times. Conventionally, sorption-desorption reactions are modeled as instantaneous equilibrium reactions according to the "linear equilibrium isotherm"[13]:

$$K_d = \frac{C_s}{C_w} \quad , \qquad (4.3\text{-}21)$$

where:

K_d - equilibrium constant or "distribution factor"; [cm^3/g],
C_s - equilibrium concentration of radionuclides affixed to the solid phase; [g^{-1}],
C_w - concentration of radionuclides in the aqueous phase; [cm^{-3}].

Adopting the above description of sorption-desorption reactions, the new expression for $\underline{J}$, the flux of species in the aqueous medium becomes:

$$\underline{J} = - D \underline{\nabla} C_w + \underline{u} C_w, \tag{4.3-22}$$

where:

$$D = D^* /R, \tag{4.3-23}$$

$$\underline{u} = \underline{u}^* /R, \tag{4.3-24}$$

and R is a dimensionless quantity, known as the "retardation factor," which is defined as follows:

$$R = 1 + K_d \rho/\varepsilon, \tag{4.3-25}$$

with ρ - bulk density of the solid phase; [g/cm^3].

Irreversible processes like radioactive decay and fixation of radionuclides into insoluble stable phases deplete the water of contaminants and reduce radionuclide migration altogether.

Taking both reversible sorption-desorption reactions and irreversible processes into consideration, conservation of aqueous species within the packing material demands that the radionuclide concentration in the aqueous phase is given by the equation:

$$\frac{\partial C_w}{\partial t} = - \underline{\nabla} \cdot \underline{J} - \lambda C_w - F(C_w, C_s), \tag{4.3-26}$$

where $\underline{J}$ is given by Eq. (4.3-22), and:

λ - radioactive decay constant; [yr^{-1}],

$F(C_w, C_s)$- equivalent rate of fixation of the given radionuclide into an insoluble stable phase; [$cm^{-3}.yr^{-1}$].

Expressions for the function $F(C_w, C_s)$ are not available. Therefore, precipitation into stable phases is not taken into account in this illustration. This leads to the following representation of the migration process:

$$\frac{\partial C_w}{\partial t} = - \underline{\nabla} \cdot \underline{J} - \lambda C_w \tag{4.3-27}$$

Equation (4.3-27) predicts higher concentrations of radionuclides than Eq. (4.3-26). Equation (4.3-27) represents the classical dispersion equation of radionuclides in porous media[10], and the reference equation for further development.

4.3.4.2 One-Dimensional Solution of the Dispersion Equation

In general, the dispersion equation, Eq. (4.4-27), requires a numerical solution, which makes parametric studies extremely expensive. It is common practice, therefore, to consider one-dimensional, linear restrictions[14,15,16] of Eq. (4.3-27). This is also based on the observation that studies of groundwater flow show that longitudinal convection and dispersion are generally greater than transverse, and that uncertainties in the input data do not warrant an overly precise description of the migration process. While these arguments are widely accepted, and a one-dimensional solution to Eq. (4.3-27) is indeed sought here, comparisons of one- and three-dimensional predictions should be thoroughly investigated, both in the linear and nonlinear cases as better data become available.

With reference to Fig. 4.3-3, consider the one-dimensional migration of radionuclides from the surface of the original waste form towards the host rock. Assuming plane geometry and a uniform groundwater flow field in the x direction, the one-dimensional, linear specialization of Eq. (4.3-27) reads:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - u \frac{\partial C}{\partial x} - \lambda C \,, \qquad (4.3\text{-}28)$$

where the subscript "w" has been dropped for simplicity. Equation (4.3-28) is accompanied with adequate initial and boundary conditions. If we set equal to zero the time at which the canister fails, and if no radionuclides are present initially in the half space $x > 0$, the initial condition is:

$$C(x,0) = 0, \quad x > 0. \qquad (4.3\text{-}29)$$

By continuity, the dispersion-convection flux at the waste form-packing material interface must be equal to the flux, L(t), due to leaching of radionuclides from the waste form. This yields the boundary condition:

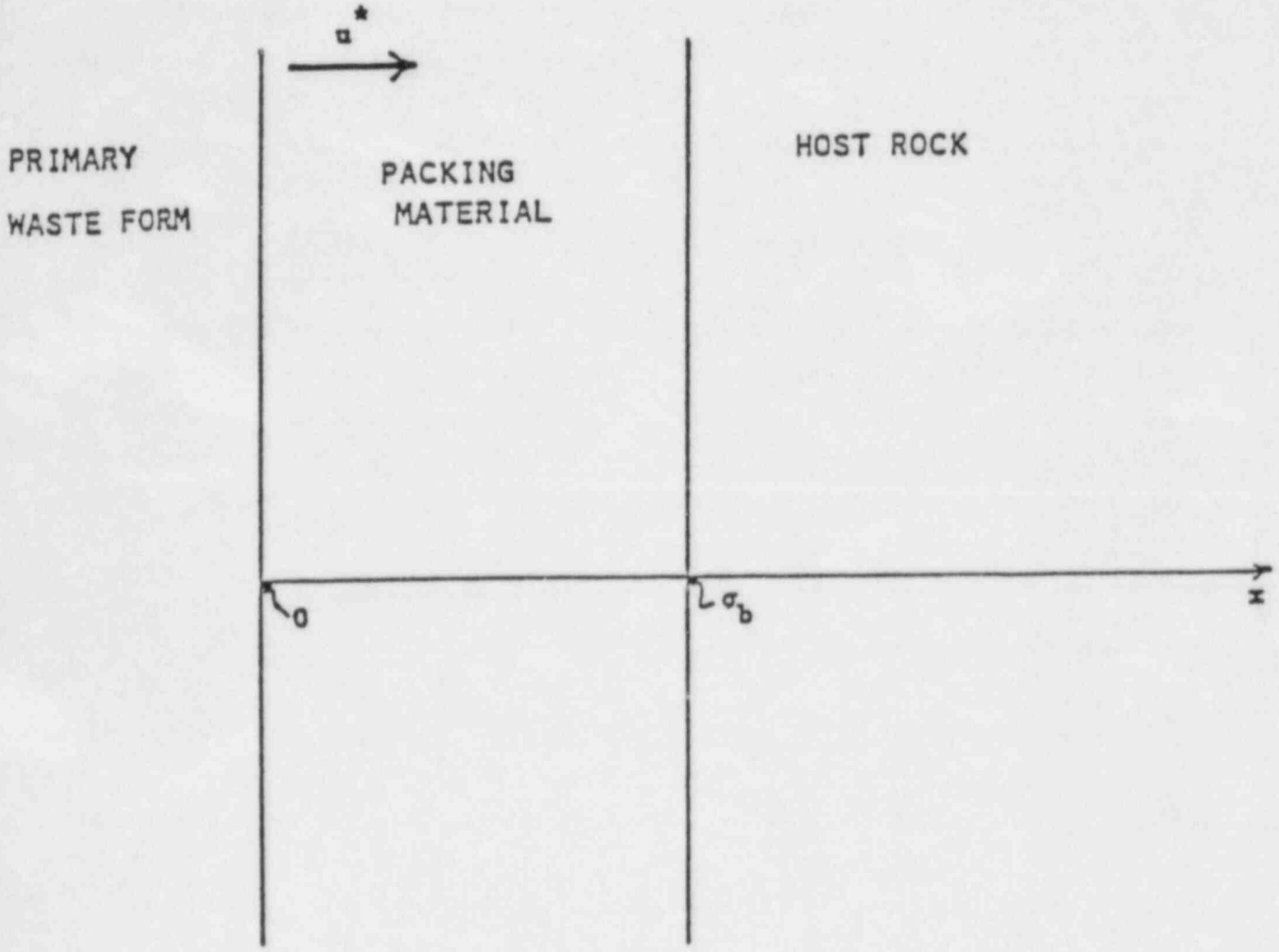

Figure 4.3-3 Schematic Representation of the Waste Form - Packing Material - Host Rock System.

$$- D\left(\frac{\partial C}{\partial x}\right)_{x=0} + uC(x=0,t) = L(t)/\varepsilon. \qquad (4.3\text{-}30)$$

In particular, if $L_o(t)$ denotes the leach rate of stable species per unit geometric surface area as it is extrapolated from short-term leaching experiments (Sect. 4.3.3), one can account for radioactive decay processes taking place within the waste form by expressing the leach rate of each parent species as follows:

$$L(t) = e^{-\lambda(t+\tau)} L_o(t) \qquad (4.3\text{-}31)$$

where τ indicates the time needed for failure of the canister. Furthermore, cracking of the original waste form "monolith" increases the effective surface area for leaching of the waste form. This effect can be taken into account by multiplying the expression for $L_o(t)$ by an adequate coefficient f of value greater or equal one. Thus the overall expression for L(t) becomes:

$$L(t) = f\, e^{-\lambda(t+\tau)} L_o(t) , \qquad f \geq 1. \qquad (4.3\text{-}32)$$

Finally, far away from the waste form it must be:

$$C(+\infty,t) = 0. \qquad (4.3\text{-}33)$$

Assuming further that the host rock poses the same resistance to radionuclide migration as the packing materials, the initial and boundary value problem describing the migration of radionuclides away from the waste form becomes:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - u\frac{\partial C}{\partial t} - \lambda C, \qquad x,t>0 \qquad (4.3\text{-}34)$$

$$C(x,0) = 0, \qquad x \geq 0 \qquad (4.3\text{-}35)$$

$$- D\frac{\partial C}{\partial x}\Big|_{x=0^+} + uC(x=0,t) = \frac{f}{\varepsilon}\, e^{-\lambda(t+\tau)} L_o(t), \qquad t \geq 0 \qquad (4.3\text{-}36)$$

$$C(+\infty,t) = 0 \qquad t \geq 0 \qquad (4.3\text{-}37)$$

Solution to the above system of equations is provided in Appendix A. The space- and time-dependent concentration of radionuclides within the aqueous phase is expressible as follows:

$$C(x,t) = \frac{f\, e^{-\lambda(t+\tau)}}{\varepsilon\, D} \int_o^t L_o(t-t')\, G(x,t')\, dt' \qquad (4.3\text{-}38)$$

where:

$$G(x,t) = \left(\frac{D}{\pi t}\right)^{1/2} \exp\left[-\frac{(x-ut)^2}{4Dt}\right]$$

$$- \frac{u}{2} \exp\left(\frac{ux}{D}\right) \operatorname{erfc}\left(\frac{x+ut}{2\sqrt{Dt}}\right), \qquad (4.3\text{-}39)$$

and the function erfc(z) is the complementary error function[17]. The analogous expression for stable species is obtained by setting $\lambda=0$.

With reference to Eq. (4.3-38), if $u\neq 0$, the following asymptotic relation holds between the radionuclide concentration at a given point and the leach rate:

$$C(x,t) \sim \frac{f\, e^{-\lambda(t+\tau)} L_o(t)}{\varepsilon\, u} = \frac{L(t)}{\varepsilon\, u}, \quad x \ll ut \qquad (4.3\text{-}40)$$

If $u = 0$, and L_o is of the form suggested in Sect. A.3.3.1:

$$L_o(t) = nK\, t^{n-1}, \qquad 0 < n < 1, \qquad (4.3\text{-}41)$$

one has for large values of the time:

$$C(x,t) \sim \frac{f\, n\, K\, \Gamma(n)\, e^{-\lambda(t+\tau)}\, t^{n-1/2}}{\varepsilon\, \Gamma(n+1/2)\, \sqrt{D}}, \quad x \ll (Dt)^{1/2} \qquad (4.3\text{-}42)$$

where $\Gamma(x)$ represents the gamma function[17].

When coupled with an expression for $L_o(t)$ and an appropriate breakthrough criterion, Eq. (4.3-38) allows a first estimate of the time interval needed for failure of the packing material to contain the migrating radionuclide.

4.3.5 A Criterion for Failure of the Packing Material During the Containment Period

If the zero release rule during the first 300 to 1,000 years after decommissioning were to be interpreted literally, all dispersion models would predict an instantaneous failure of the packing material at the same time as the canister fails. Indeed, because of the nature of Eq. (4.3-27), any disturbance to the initial condition is predicted to be propagated at infinite velocity in the dispersing medium, and the initial pulse of radionuclides at time $t = 0$ would spread out instantaneously to the boundary of the medium. In the absence of a regulatory criterion to determine failure of the waste package to contain the stored radionuclides for 300 to 1,000 years after decommissioning of the repository, the following breakthrough criterion has been selected for the sake of illustration. Namely, with reference to Fig. 4.3-2, failure is assumed to take place at a time t_f when the radionuclide release rate at the interface of the packing material with the host rock is greater than 10^{-8} parts per year of the inventory of the specific radionuclide in the waste package. Mathematically this is expressed as follows:

$$J \cdot \varepsilon / W > 10^{-8}, \quad yr^{-1} \tag{4.3-43}$$

where the quantity W indicates the total amount of material available for leaching per square centimeter of initial waste form surface. An alternative criterion could have been chosen by selecting W as the total amount of material available for leaching per square centimeter of waste form surface after 1,000 years emplacement.

4.3.6 A Criterion for Failure of the Packing Material During the Controlled Release Period

Following the containment period, waste package failure occurs, according to 10 CFR 60, when the radionuclides transfer rate per unit area, J, from the waste package to the host rock is high enough to cause the engineered barrier system to release more than one part in one hundred thousand per year of the stored radionuclides assuming no release. A critical value for J can be

obtained only in a wider scope analysis which factors in properties of the engineered barriers and of the repository system. However, in order to proceed with this illustration of Monte Carlo analysis, failure is conservatively assumed to take place at a time t_f when the radionuclides transfer rate at the interface of the packing material with the host rock is greater than 10^{-5} parts per year of the inventory of the specific radionuclide in the waste package assuming no release. Mathematically, this is expressed as follows:

$$J\ \varepsilon/W > 10^{-5},\ yr^{-1} \qquad (4.3\text{-}44)$$

where the quantity W indicates the total amount of material available for leaching after 1,000 years per unit area of initial waste form surface, assuming no release. In particular, since the isotopes considered for this illustration have very long half-lives, the quantity W was considered to be unchanged, for calculational purposes, during the first 1,000 years after emplacement. This introduces negligible error in the calculations.

4.4 Computer Program

A computer program incorporating the thermal, corrosion and leaching-transport models has been written for the repetitive computation of cases with inputs which vary according to the prescribed distributions. The program incorporates as a sub-program the SANDIA program LHC which generates the sample of cases using a Latin Hypercube scheme (SAND-79-1473;1980). In the present implementation, any of the input parameters can be assigned a distribution type and ranges over which LHC will generate the values for the samples. The name of the program is WASTE and can be obtained from the Division of Nuclear Waste Management at Brookhaven National Laboratory.

4.5 Results

Using the input values shown in Table 4.5-1, the program was run for 476 cases.

Table 4.5-1 Input Data

Canister Temperature Input Data

I	Decay Constants (1/year)	Fractional Power
1	1.0000000E+00	-9.5152900E-02
2	3.3333000E-01	3.1726500E-01
3	1.1111100E-01	-3.3085700E-01
4	3.7037000E-02	9.4509600E-01
5	1.2345600E-02	1.3584500E-01
6	4.1152300E-02	-4.6195500E-03
7	1.3717400E-03	2.4842000E-02
8	4.5725000E-03	-3.3234500E-03
9	1.5242000E-04	2.4997200E-03
10	5.0810000E-05	2.0536900E-03

	Lower 0.001 Quantile	Upper 0.001 Quantile	Distribution Function
Rock Properties			
Geothermal Temperature (C)	54.0000	60.0000	Uniform
Thermal Conductivity (W/M/K)	1.2500	2.5000	Uniform
Density (KG/CU.M)	2410.0000	2800.0000	Uniform
Specific Heat (J/KG/K)	820.0000	1160.0000	Uniform
Emplacement Geometry			
Pack Density (1/M/M)	0.00748	0.00000	Linear
Waste Package Parameters			
Waste Age (Years)	0.0000	0.0000	Linear
Initial Power (KW)	2.1000	0.0000	Linear
Rock Shell Thermal Conductivity (W/M/K)	1.2500	2.5000	Uniform
Outer Diameter of Backfill (M)	0.6860	0.0000	Linear
Thermal Conductivity of Backfill (W/M/K)	0.4000	1.4000	Uniform
Outer Diameter of Overpack (M)	0.3250	0.0000	Linear
Thermal Conductivity of Buffer (W/M/K)	10.0000	0.0000	Linear
Outer Diameter of Canister (M)	0.3250	0.0000	Linear
Canister Thickness (M)	0.0530	0.0000	Linear
Length of Canister (M)	4.1000	0.0000	Linear

Table 4.5-1 (Continued)

Canister Temperature Input Data	Lower 0.001 Quantile	Upper 0.001 Quantile	Distribution Function
Pitting Factor	1.0000	6.0000	Uniform
Exponent of Time	0.3639	0.5736	Normal
Uniform Corrosion Coefficient (MM/YR)	0.0015	676.0000	Lognormal
Chlorine (PPM)	1.0000	100.0000	Uniform
Oxygen (PPM)	0.0100	3.0000	Uniform
Leaching Input Data			
Hydraulic Conductivity (CM/YR)	0.0001	0.3000	Uniform
Hydraulic Gradient	0.0050	0.0300	Uniform
Density (GM/CM**3)	2.1000	2.7000	Uniform
Porosity	0.0010	0.0000	Linear
Exponent of Time	0.1000	0.7500	Uniform
Leach Rate Factor≠ X	3.1800	0.0000	Linear
Leach Rate Factor≠ Y	-2424.2200	0.0000	Linear
Leach Rate Factor≠ Z	-0.4000	0.4000	Uniform
Density of Glass (GM/CM**3)	3.0000	0.0000	Linear
Radius of Glass (CM)	30.5000	0.0000	Linear
Crack Factor of Glas	2.0000	40.0000	Uniform
Plutonium			
Distribution Factor (CM**3/GM)	45.0000	5200.0000	Lognormal
Diffusivity (CM**2/YR)	3.1500	315.0000	Uniform
Dispersivity (CM)	0.0000	1525.0000	Uniform
Technetium			
Distribution Factor (CM**3/GM)	0.0000	0.0000	Linear
Diffusivity (CM**2/YR)	3.1500	315.0000	Uniform
Dispersivity (CM)	0.0000	1525.0000	Uniform

≠Eq. (4.3-19b) in text.

Table 4.5-2 shows a summary the results. There were nine cases showing failure of the canister due corrosion in less than 1000 years. All cases showed failure of containment Technetium and one of the cases showed failure of containment for Plutonium Failure to meet the controlled release criterion occurred in 10 cases.

From the results of 476 cases, probability of failing the containment criterion is 2%. The probability of iling the controlled release criterion is also 2%. This does not mean tha is expected that 2% of the canisters in a repository constructed accordin this design will fail, but means that there is a 2% chance that all the ca ters will fail since the causes of the uncertainty are common to all caniste

Inspection of the time to failu data shows that the failures tend to occur early, if they occur at all. s is due to the combined effect of the early high temperatures and of the reasing rate of corrosion with time. The presence of the packing materia ppears to be beneficial for plutonium but shows no significant benefit for chnetium. The dominant uncertainty in the time to failure is introduced by e uncertainty of the overall corrosion coefficient.

Table 4.5-2

Monte Carlo Results

Case #	Time of Can Failure years	Technetium Fract. Release per year	Plutonium Fract. Release per year
1 - 6	5162	8.4 E-7	1.4 E-30
1 -11	72	4.8 E-4	4.4 E-40
1 -52	27	8.6 E-5	1.4 E-14
1 -83	2376	1.2 E-5	2.1 E-5
1 -94	4648	NA	1.2 E-10
2 - 8	2808	4.6 E-9	3.0 E-22
2 -14	9700	5.5 E-8	2.3 E-279
2 -56	7220	5.6 E-5	2.3 E-9
3 - 8	918	6.3 E-6	3.8 E-17
3 -17	5696	4.5 E-8	3.8 E-15
3 -34	7760	3.2 E-7	1.9 E-17
3 -55	7	4.0 E-4	3.2 E-23
4 - 4	611	8.7 E-7	8.3 E-10
4 -20	308	1.2 E-5	1.7 E-17
4 -21	35	6.1 E-2	4.5 E-8
5 -16	18	3.3 E-2	3.3 E-6
5 -27	18	1.0 E-1	6.6 E-27
5 -38	3300	6.1 E-8	1.7 E-11
5 -40	2310	1.3 E-5	3.3 E-7
5 -82	4482	NA	3.3 E-13

5. CONCLUSIONS

Probabilistic Reliability Analysis affords a disciplined approach toward addressing the inherent reliability of a system and provides valuable insight into the system weaknesses and strong points. As such, it works to the advantage of both the regulator, in his evaluation of the quality of the submitted evidence, and of the applicant during various stages of the design project.

Probabilistic Reliability Analysis has been used before by the nuclear industry to demonstrate power plant performance in compliance with pertinent criteria within the framework of the applicable NRC standards of reasonable assurance. This has led to a continuous refining of the techniques with each new application to nuclear power plant analysis.[2]

This document proposes the general method of probabilistic reliability analysis as an acceptable framework to identify, organize and convey the necessary information to satisfy the standard of reasonable assurance of waste package performance according to the regulatory requirements during the containment and controlled release periods. Based on available guidelines from References [2] and [3], suggested requirements for reliability analysis have been proposed. In particular, the analysis should be subdivided into two complementary parts encompassing qualitative and quantitative elements respectively. Qualitative analysis provides an identification of the various failure modes that contribute to waste package unreliability; quantitative analysis utilizes available experience on waste package components and their interactions and provides a numerical value of the probability that the waste package will perform its intended mission.

The proposed, main operational tool of qualitative reliability analysis is the failure modes and effects analysis - FMEA. This should be an integral part of the early design evaluation and should be periodically updated to reflect changes in design or application.

The core of quantitative reliability analysis is the uncertainty analysis which deals with the quantification of uncertainties in parameters, models, and in the degree of completeness of the implemented approach as well as the propagation of the uncertainties in the analysis. While it is recognized that uncertainty analysis lacks mathematical rigor, it is nevertheless recognized that it offers valuable tools in decision making, as testified by its use in the licensing of commercial nuclear power plants. In particular this document shows that at least one technique exists - namely, Monte Carlo simulation - for uncertainty propagation and for calculating the probability of a waste package to perform its intended mission.

This document does not show how to address uncertainties in model applicability or degree of completeness of the analysis, which may require a survey of expert opinions. Guidance on this topic is provided by Reference [2]. In particular, Reference [2] notes the dichotomy between the subjective or Bayesian approach to uncertainty analysis and the classical or frequentist one. We would suggest that the present document be used as a stepping stone to explore those wider issues.

APPENDIX A

SOLUTION TO THE INITIAL AND BOUNDARY VALUE PROBLEM EQS. (4.3-34) THROUGH (4.3-37).

With reference to the initial and boundary value problem represented by Eqs. (4.3-34) through (4.3-37), it proves convenient to make the transformation of the independent variable:

$$C(x,t)\,\frac{\varepsilon}{f} = N(x,t)\,e^{-\lambda t}. \tag{A.1}$$

In terms of the new function $N(x,t)$ the original problem takes on the simpler form:

$$\frac{\partial N}{\partial t} = D\,\frac{\partial^2 N}{\partial x^2} - u\,\frac{\partial N}{\partial x}, \qquad x,t>0, \tag{A.2}$$

$$-D\,\frac{\partial N}{\partial x}\Big|_{x=0^+} + N(x=0,t) = e^{-\lambda\tau}\,L_o(t), \qquad t \geq 0, \tag{A.3}$$

$$N(\infty,t) = 0, \qquad t \geq 0, \tag{A.4}$$

$$N(x,0) = 0, \qquad x \geq 0. \tag{A.5}$$

Taking the Laplace transform of Eqs. (A.2) through (A.5), the new system of equations in terms of the transformed functions $N(x,p)$ and $L_o(p)$ becomes:

$$p\,\bar{N} = D\,\bar{N}'' - u\,\bar{N}', \qquad x > 0, \tag{A.6}$$

$$-D\,\bar{N}'(x=0,p) + u\,\bar{N}(x=0,p) = e^{-\lambda\tau}\,\bar{L}_o(p), \tag{A.7}$$

$$\bar{N}(\infty) = 0, \tag{A.8}$$

where p is the parameter of the transformation and a prime indicates ordinary differentiation with respect to the space variable x. Equation (A.6) admits the general solution:

$$\bar{N}(x,p) = u\,e^{\gamma_1 x} + \upsilon e^{\gamma_2 x}, \tag{A.9}$$

where the two parameters γ_1 and γ_2 are defined as follows:

$$\gamma_1 = \frac{u + (u^2 + 4pD)^{1/2}}{2D} , \tag{A.10}$$

$$\gamma_2 = \frac{u - (u^2 + 4pD)^{1/2}}{2D} , \tag{A.11}$$

Choosing to operate on the main branch of the square root function, defined by the relation:

$$-\pi < \arg\left(p + \frac{u^2}{4D}\right) \leq \pi, \tag{A.12}$$

it turns out that:

$$\mathrm{Re}\,[\gamma_1] > 0, \tag{A.13}$$

and

$$\mathrm{Re}\,[\gamma_2] < 0. \tag{A.14}$$

Therefore, the particular solution of Eq. (A.6) which is of interest to us takes on the form:

$$\bar{N}(x,p) = \mu(p)\, e^{-\xi(p)x}, \qquad x > 0 \tag{A.15}$$

where

$$\xi(p) = -\gamma_2. \tag{A.16}$$

The function $\mu(p)$ can be obtained by combining the boundary condition Eq. (A.7) and Eq. (A.15) together. It turns out:

$$\mu(p) = \frac{e^{-\lambda\tau}\, \bar{L}_o(p)}{D\,\xi(p) + u} , \tag{A.18}$$

and, one can rewrite Eq. (A.15) as follows:

$$\bar{N}(x,p) = \bar{F}(p) \cdot G(\bar{x},p), \tag{A.18}$$

where:

$$\bar{F}(p) = \frac{e^{-\lambda\tau}\, \bar{L}_o(p)}{D} , \tag{A.19}$$

and

$$\bar{G}(x,p) = \exp\left(\frac{ux}{2D}\right) \cdot \frac{\exp\left[-\left(\frac{u^2}{4D^2} + \frac{p}{D}\right)^{1/2} x\right]}{\left(\frac{u^2}{4D^2} + \frac{p}{D}\right)^{1/2} + \frac{u}{2D}} . \tag{A.20}$$

By a property of the Laplace transforms, the function N(x,t) can be expressed as the convolution of the original functions F(t) and G(x,t). Namely:

$$N(x,t) = \int_0^t F(t-t')\, G(x,t')\, dt'. \tag{A.21}$$

The function $\bar{F}(p)$ is easily inverted yielding:

$$F(t) = \frac{e^{-\lambda\tau} L_o(t)}{D} . \tag{A.22}$$

In order to invert the function $\bar{G}(x,p)$, one can observe that it is of the form:

$$\bar{G}(x,p) = \exp\left(\frac{ux}{2D}\right) \bar{H}\left(\frac{p}{D} + \frac{u^2}{4D^2}\right) , \tag{A.23}$$

Therefore, its inverse must be of the form:

$$G(x,t) = D \exp\left(\frac{u^2 t}{4D} + \frac{ux}{2D}\right) . H(Dt) \tag{A.24}$$

where

$$H(t) = \mathcal{L}^{-1}\left\{\bar{H}(p)\right\}$$

$$= \mathcal{L}^{-1}\left\{ \frac{\exp\left(-\sqrt{p}\, x\right)}{\sqrt{p} + \frac{u}{2D}} \right\} \tag{A.25}$$

It turns out, from the tables, that:

$$H(t) = \left(\frac{1}{\pi t}\right)^{1/2} \exp\left(-\frac{x^2}{4t}\right)$$

$$- \frac{u}{2D} \exp\left(\frac{ux}{2D} + \frac{u^2 t}{4D^2}\right) \operatorname{erfc}\left(\frac{u\sqrt{t}}{2D} + \frac{x}{2\sqrt{t}}\right) \tag{A.26}$$

Therefore, combining the above results, the function N(x,t) is expressible as follows:

$$N(x,t) = \frac{e^{-\lambda\tau}}{D} \int_0^t L_o(t-t')\, G(x,t')\, dt', \qquad (A.27)$$

where:

$$G(x,t) = \left(\frac{D}{\pi t}\right)^{1/2} \exp\left[-\frac{(x-ut)^2}{4Dt}\right] \qquad (A.28)$$

$$- \frac{u}{2} \exp\left(\frac{ux}{D}\right) \operatorname{erfc}\left(\frac{x+ut}{2\sqrt{Dt}}\right)$$

Combining Eq. (A.27) and Eq. (A.1) together, the reported expression for C(x,t), Eq. (4.3-38), follows.

APPENDIX B

TEMPERATURE MODEL

With reference to Figure 4.3.1 and to the consideration of Section 4.3.1, this appendix describes how a temperature model could be developed. Modeling of the decay heat is accomplished first in Section B.1. The resulting expression is then used to develop a far field temperature model in Section B.2. Treatment of the near field region is accomplished in Section B.3. Model validation, and data for the temperature model are addressed in Section B.4 and B.5, respectively.

B.1 POWER GENERATION MODEL

The parameters which determine the power as a function of time for a single waste package are the age of the waste and the type of fuel which originated it, as well as the loading of waste into the individual waste package.

The age and the type of the waste enter into the details of the decay curve, and the loading of the glass enters as a multiplier.

It is assumed that the power dissipation of the waste can be represented as

$$P = P_o \sum_{i=1}^{n} a_i \, e^{-\lambda_i t} \qquad \text{(B.1-1)}$$

where the set of a_i is normalized so that P_o is the power at t=0 and t is the time since reprocessing.

The values of λ_i and a_i can be obtained by least square fitting procedure to data produced by a fission product decay code such as ORIGEN, with appropriate corrections for the efficiency of recovery of the various elements. For example, the contribution to the power from the noble gases should be negligible, and the volatile fission products which are not retained in the glass need to be reduced proportionately.

The decay constants λ_i can be determined from the fit of the computed results in which case they will resemble the natural decay constant of the dominant fission and activation products, or alternatively they can be taken

arbitrarily in a logarithmic sequence which spans the range of natural decay constants. In any case the justification of the choice of the set of λ_i and a_i rests on the accuracy of the fit to the results of a detailed fission and activation product calculation which includes all the significant isotopes.

The expression for the power is modified to shift the origin of time to the age of the waste at the time of emplacement in the repository. If the age of the waste is t_o, then

$$P = P_o \sum_{i=1}^{n} a_i \, e^{-\lambda_i (t+t_o)} \qquad (B.1\text{-}2)$$

where t is now measured from emplacement time.
Then,

$$P = P_o \sum_{i=1}^{n} a_i \, e^{-\lambda_i t_o} \cdot e^{-\lambda_i t} = P_o \sum_{i=1}^{n} b_i \, e^{-\lambda_i t} \, . \qquad (B.1\text{-}3)$$

The power after emplacement, P, normalized to the power at emplacement time P_i can be expressed as:

$$\frac{P}{P_i} = \frac{\sum_{i=1}^{n} b_i \, e^{-\lambda_i t}}{\sum_{i=1}^{n} b_i} = \sum_{i=1}^{n} c_i \, e^{-\lambda_i t} .$$

The temperature of the repository resulting from the overall heat conduction of the rock formation depends on the average heat generation per unit area of repository, and this average heat generation can be represented by

$$Q(t) = m \, P_i \sum_{i=1}^{n} c_i \, e^{-\lambda_i t} \qquad (B.1\text{-}4)$$

where:

- $Q(t)$ = Power per unit area of Repository [W/m^2],
- m = Average number of waste packages per unit area of repository [$1/m^2$],
- P_i = Power per package at emplacement time [W],
- t = Time from emplacement [year],
- λ_i = Decay constant of isotope group i [$year^{-1}$], and
- c_i = Fraction of power due to isotope group i at emplacement time [dimensionless].

B.2 FAR FIELD TEMPERATURE MODEL

With reference to Fig. 4.3.1, it is assumed that the repository is an extended plane heat source immersed in an infinite homogeneous medium initially at constant temperature. The only temperature of interest is that of the plane source.

According to the considerations of Section B.1, the heat source per unit area is taken to be a function of the form:

$$f(t) = \sum_{i=1}^{n} a_i \, e^{-\lambda_i t}, \qquad (B.2\text{-}1)$$

where n is the number of isotopes groups, λ_i their decay constants and a_i coefficients for each isotope in units of cal/sec/sq meter, and depend on parameters such as dimensions of the glass block, percent loading, age of the waste, and density of emplacement on the repository floor.

From Carslaw and Jaeger, p.76, assuming heat conduction in a semi-infinite solid, the temperature at the source is:

$$T = \frac{\sqrt{k}}{K\sqrt{\pi}} \int_0^t f(t-z) \, \frac{dz}{\sqrt{z}} + T_o \qquad (B.2\text{-}2)$$

where:

T = Temperature at time t,

K = Thermal conductivity,
k = Thermal diffusivity = $\frac{K}{\rho c}$,

ρ = Density,

c = Heat capacity,

z = Dummy time variable in any consistent set of units, and

T_o = Initial, background geothermal temperature.

Since in the real case, the heat flows in two directions, up and down, equation (B.2-2) has to be changed to:

$$T = \frac{\sqrt{k}}{2K\sqrt{\pi}} \int_0^t f(t-z) \, \frac{dz}{\sqrt{z}} + T_o \qquad (B.2\text{-}2)$$

Combining Eqs. (B.2-1) and (B.2-3) one obtains:

$$T = \frac{\sqrt{k}}{K\sqrt{\pi}} \sum_{i=1}^{n} \frac{a}{\sqrt{\lambda_i}} \Delta(\sqrt{\lambda_i t}) \ , \qquad (B.2\text{-}4)$$

where, the function $\Delta(x)$ is the Dawson's integral defined as:

$$\Delta(x) = \exp(-x^2) \int_0^x \exp(+t^2)\, dt. \qquad (B.2\text{-}5)$$

Therefore, the far field effect on the repository center plane can be expressed as a sum of terms, each of which requires the evaluation of a single transcendental function, the Dawson's integral.

B.3 NEAR FIELD TEMPERATURE MODEL

To compute the local temperature rises in the vicinity of the canister, the assumption is made that the problem can be treated as a one-dimensional steady-state radial heat conduction through concentric layers. In order to match the local solution with the far field solution, the outer surface of the outer shell corresponding to one canister length is made equal to the horizontal area of repository per canister. Then the outer radius of the equivalent rock shell is

$$R = \frac{d}{\pi} \qquad (B.3\text{-}1)$$

where

d = distance between parallel emplacement holes.

The adopted model, which is based on steady-state elementary heat conduction considerations in concentric cylindrical geometry, accepts three shells, eg. near rock, packing material (backfill) and buffer, and requires the corresponding diameters, and the thermal conductivities.

B.4 MODEL VALIDATION

In order to validate this model, several three-dimensional solutions of the heat conduction problem should be compared with the results of the model, to estimate the expected errors of prediction. It is expected that errors would tend to be systematic since the matching of the two solutions overestimates the temperature, because the thermal inertia of the near rock is neglected. Therefore, if there are enough points to compare the results, a correction function could be introduced.

The results of this simplified model, adjusted for an outer diameter of the rock shell that would represent the case of vertical emplacement holes having only one canister per hole, were compared with the results reported in NWTS-16, "Interim Reference Repository Conditions for a Nuclear Repository in Basalt," for the case of spent fuel. The results for canister temperatures were found to agree with the published results within 20°C, however, it is not possible to separate errors due to the approximations made in the model from differences between input data sets.

For an actual validation of the simplified model, the results should be compared with a series of cases where the actual values of the parameters used in both calculation are known.

B.5 TEMPERATURE MODEL DATA

Data for the relative decay heat generation as a function of time is taken from the draft NWTS-16, "Interim Reference Repository Conditions for a Nuclear Waste Repository in Basalt," where the data is presented in tabular form for periods of 0 to 9990 years after emplacement. Emplacement is assumed to occur 10 years after reactor discharge. The data for "Commercial High-Level Waste" is used in this document. This data assumes a 3:1 mix of UO_2 and mixed oxide fuels.

Decay heat data are expected to have two sources of uncertainty: the details of the fuel cycle that produced the waste, and the details of the chemical reprocessing which allow certain latitude in the fraction of actinides re-

covered. At later times, when most of the heat generated results from the decay of the actinides these uncertainties can be substantial.

Disregarding these uncertainties, the above set of data is taken as exact, and the data are fitted to a sum of exponential functions. The resulting set of decay constants and factors is shown in Table B.5-1. The decay constants are not adjusted in the fit but are fixed in a geometric scale of factor 0.3333. Some improvement on the fit could be obtained by a non-linear fit where the decay constants are taken as unknowns, but the gains are judged not to warrant the additional complication. Table B.5-2 shows the decay-heat data, the predictions of the fit, and the fractional error of the fit. Figure B.5-1 shows a plot of the results.

Since the data used for this fit are normalized to 10 years after discharge, and a few years does not appear to affect the results substantially, the input for the age of the fuel in the model is fixed at a point estimate value of 10 years. In the program this is implemented by entering a zero age. The performance model accommodates variable ages of the waste only if the data is normalized to zero age.

The geothermal temperature given in the BWIP-SCR, p. 6.2-6, shows a spread of about 5 degrees. Therefore, for a nominal temperature of 57 degrees centigrade, the adopted range is 54 to 60 degrees.

The thermal properties, specific heat and thermal conductivity of the basalt of the Umtanum flow are taken from the BWIP-SCR (Table 4.9), where the data are presented in the form of a range of values but without a detailed analysis or statements about probability distribution type and parameters. For the purposes of this illustration, the thermal conductivity is assumed to be uniformly distributed in the range 1.25 to 2.50 W/m°K and the specific heat also uniformly distributed in the range 820 to 1160 J/kg°K.

The basalt density is taken from BWIP-SCR (Tables 4.6 and 4.7) where the data shown exhibits a range of 2410 to 2800 kg/cu.m. For the purpose of this illustration, the thermal properties and the density are taken as independent

Table B.5-1

Decay Heat Source Regression Results

Term #	Decay Constant [1/year]	Coefficient [-]
1	1.00000000	-0.09515290
2	0.33333300	0.31726500
3	0.11111100	-0.33085700
4	0.03703700	0.94509600
5	0.01234570	0.13584500
6	0.00411523	-0.00461955
7	0.00137174	0.02484200
8	-0.00045725	-0.00332345
9	0.00015242	0.00249972
10	0.00005081	0.00205369

Table B.5-2

Decay Heat Data and Results

Time	Power Data	Power Predict.	Fractional Error
0.00	1.000000	0.993648	0.006352
1.00	0.950000	0.962611	-0.013275
2.00	0.907000	0.916657	-0.010647
3.00	0.871000	0.872934	-0.002220
4.00	0.851000	0.835403	0.018327
5.00	0.810000	0.803875	0.007562
6.00	0.783000	0.777121	0.007508
7.00	0.769000	0.753884	0.019656
8.00	0.734000	0.733144	0.001166
9.00	0.714000	0.714144	-0.000201
10.00	0.692000	0.696345	-0.006279
15.00	0.600000	0.616018	-0.026696
20.00	0.529000	0.542423	-0.025374
0.00	0.402000	0.414147	-0.030215
40.00	0.313000	0.314709	-0.005458
50.00	0.246000	0.241042	0.020155
70.00	0.157000	0.148228	0.055874
100.00	0.086400	0.082727	0.042509
190.00	0.029600	0.032286	-0.090749
290.00	0.021500	0.020599	0.041910
390.00	0.016300	0.016312	-0.000715
490.00	0.014500	0.014057	0.030572
590.00	0.012700	0.012484	0.016970
690.00	0.011300	0.011207	0.008222
790.00	0.010000	0.010107	-0.010741
890.00	0.008970	0.009145	-0.019483
990.00	0.008100	0.008300	-0.024661
1990.00	0.004040	0.003983	0.014029
5990.00	0.002300	0.002310	-0.004320
9990.00	0.001750	0.001747	0.001673

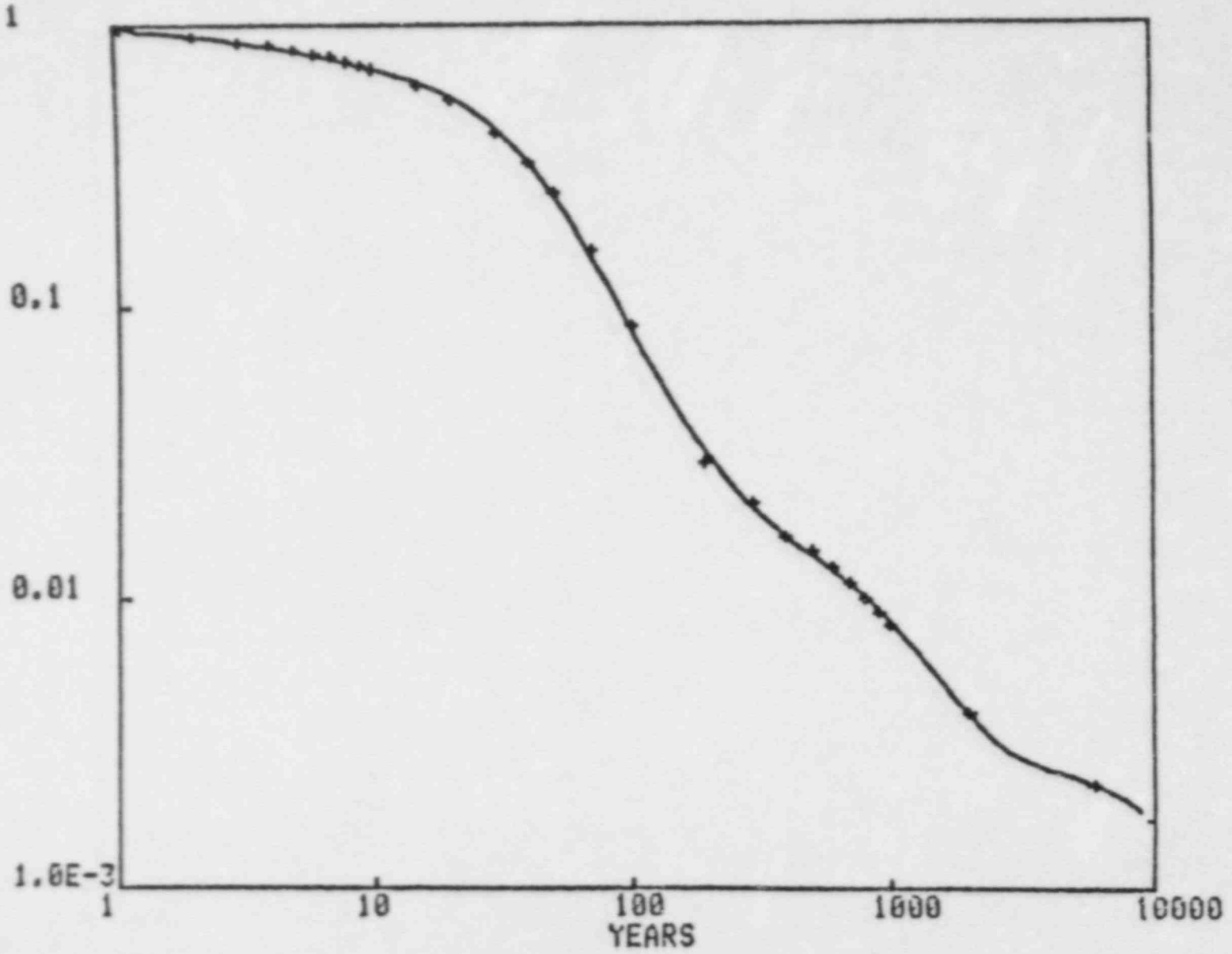

Figure 8.5-1 **Fit To Decay Heat Data For Commercial Waste.**

variables which is not correct. Since this data is used in the heat conduction equation, a more realistic treatment would be to use as the input the thermal diffusivity with its appropriate range or alternatively, to use the density, thermal conductivity and specific heat with the observed values of correlation between them.

The decay heat per canister at the time of emplacement is one of the design variables which can be adjusted to control the peak temperatures, and is subject to quality control during fabrication of the waste form. For commercial high level waste, the BWIP-SCR uses the design basis value of 2210 W/-canister. For this illustration, this value is taken without uncertainty. The uncertainty of this parameter will depend on quality control limits to be determined.

The repository design described in BWIP-SCR uses an arrangement of multiple horizontal holes at a pitch of 32.6 m. This figure and the canister length of 4.1 m leads to a packing density of 0.00748 canisters/sq.m. This value overestimates the heat loading used in the far field temperature since it neglects spacing between canisters, galleries and unused spaces at the end of emplacement holes. Since this parameter is well defined and controllable, it is taken as a point estimate without range.

The BWIP-SCR gives the following dimensions for the waste package for commercial high level waste: diameter of storage hole 0.686 m, outside diameter of canister 0.325 m, canister wall thickness 0.053 m.

The thermal conductivity of the basalt-bentonite packing material has substantial uncertainties which include effects of hydration and swelling. Altenhofen[20] gives values for bentonite and bentonite-crushed basalt ranging from 0.4 to 1.4 W/m.K depending on water content.

A summary of the thermal data for the temperature descriptive model is presented in Table B.5-3.

Table B.5-3

Summary of Data for Package Temperature Model

	Range	Distribution
Geothermal temperature [°C]	54,60	Uniform
Rock thermal conductivity [W/m/°K]	1.25,2.50	Uniform
Rock Density [Kg/cu.m]	2481,2800	Uniform
Heat Capacity [J/Kg/°K]	820,1160	Uniform
Packing Density [1/m/m]	0.00748,0.00748	----
# Age of the Waste [year]	0,0	----
Initial Decay Heat per Canister [W]	2210	----
Outer Diameter of Backfill [m]	0.686,0.686	----
Packing Material Thermal Conductivity [W/m/°K]	0.4, 1.4	Uniform
*Outer Diameter of Overpack [m]	0.325,0.325	----
*Buffer Thermal Conductivity [W/m/°K]	10,10	
Thickness of Canister [m]	0.053,0.053	----
Outer Diameter of Canister [m]	0.325,0.325	----
Length of Canister [m]	4.1,4.1	----

*Dummy values to accommodate lack of overpack.

#An input of zero for the age of the waste corresponds to 10 years after discharge, because of the normalization of the decay heat function.

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Probabilistic Reliability Analysis is identified as the preferred method to identify, organize, and convey the necessary information to meet the NRC standard on reasonable assurance of waste package performance according to regulatory requirements. The document addresses both the qualitative and quantitative aspects of the analysis, and suggests reliability analysis requirements by a prospective license applicant as well as review procedures by the regulatory agency. In particular, a method for the quantitative evaluation of a waste package reliability is demonstrated through a simplified analysis. The method is based on the repetitive usage of a performance model for values of the model parameters that span their range of uncertainty. Techniques for selecting values of the input parameters, viewed as random variables, and for generating empirical correlations among experimental data are also described. Aspects which would need to be covered in a more comprehensive document are indicated.

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